

1663

Electron Communities

The Next Mars Rover

What's Lacking with Fracking

Mini Satellites with Mega Payoff



Our antibiotics are failing. Now what?

The Curiosity rover has been traversing Mars's surface for over three years. This self-portrait is a composite of many images that were taken in one day by the Mars Hand Lens Imager (MAHLI) camera, which sits atop a turret at the end of a long robotic arm. When the images were digitally stitched together, most of the arm was removed. The next Mars rover will launch in 2020, bearing several key instruments designed and built at Los Alamos. Building upon Curiosity's atom-recognizing instrument suite, the new rover will be able to tell what molecules, and therefore which geological minerals, make up the rocks of the Red Planet. See "Getting to Know Our Neighbors," on page 16.

CREDIT: NASA/JPL-Caltech, Malin Space Science Systems, James Sorenson



About the Cover:

De-funct (di-funkt') *adj.* No longer in effect or use. Antibiotics revolutionized the treatment of infectious disease in the mid-1900s, but many no longer work, and resistant bacteria pose a significant threat to global populations. According to the World Health Organization, an era in which common infections and minor injuries could kill is a very real possibility for the 21st century. Although the use—and misuse—of antibiotics is a significant cause of antibiotic resistance, there has also been a decline in new drug development over the last few decades, compounding the severity of the current situation. Los Alamos scientists have developed a new drug pipeline to screen for new drug candidates and rapidly produce the drugs in the lab. They have already identified two new candidates, which may ultimately be available in a pharmacy near you.

About Our Name:

During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

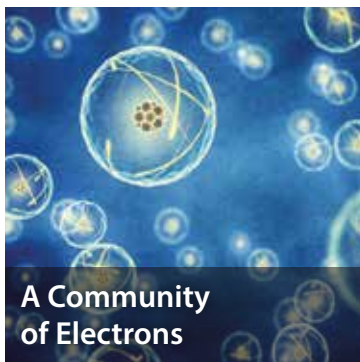
About the LDRD Logo:

Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.

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A Community of Electrons

When Los Alamos scientists solved the decades-long mystery of plutonium's missing magnetism, they got more than they bargained for: a groundbreaking insight into the overall nature of matter.

PLUTONIUM OUGHT TO PRODUCE MAGNETISM.

Physicists and physical chemists have known this for more than 50 years. The orbital motion and intrinsic spin of electrons in plutonium atoms should conspire to create tiny loops of electrical current like miniature electromagnets. These should line up in an ordered array of magnetic atoms to make the material magnetic overall. Indeed, convincing theories have emerged to explain all six of solid plutonium's allotropes—sub-phases arising at different temperatures, each with its own distinct appearance and behavior—and those theories, too, provide for overall magnetism. All of this would make for a lovely scientific success story if plutonium metal were actually magnetic.

Instead, experiment after experiment shows the same thing: no detectable magnetic order. For more than half a century, this missing magnetism has remained a troubling curiosity. After all, here is an element of tremendous importance to nuclear weapons and several other essential technologies, which the government goes to great lengths to master in every detail, and yet, decade in and decade out, the best minds in the business are forced to go about their work with the nagging certainty that they've got something manifestly wrong.

Still, there's no need to duck and cover until a credible authority on plutonium says it's safe to come out—or even if there had been such a need, there isn't any more. The Los Alamos and Oak Ridge national laboratories and external collaborators have put forth new research, referred to by the Program Chair for the last international Plutonium Futures conference as “the most significant measurement on plutonium in a generation,” resolving the missing-magnetism problem. The result is certain to benefit plutonium applications in important ways. Yet it is also broader than that. It is the key to a deeper understanding of other complex elements and compounds with distinctive electronic properties, and as such, it opens the door to a new era of advanced materials.

Beyond the simple solid

The standard lore taught to chemistry students goes like this: As you work your way down and across the periodic table, atoms

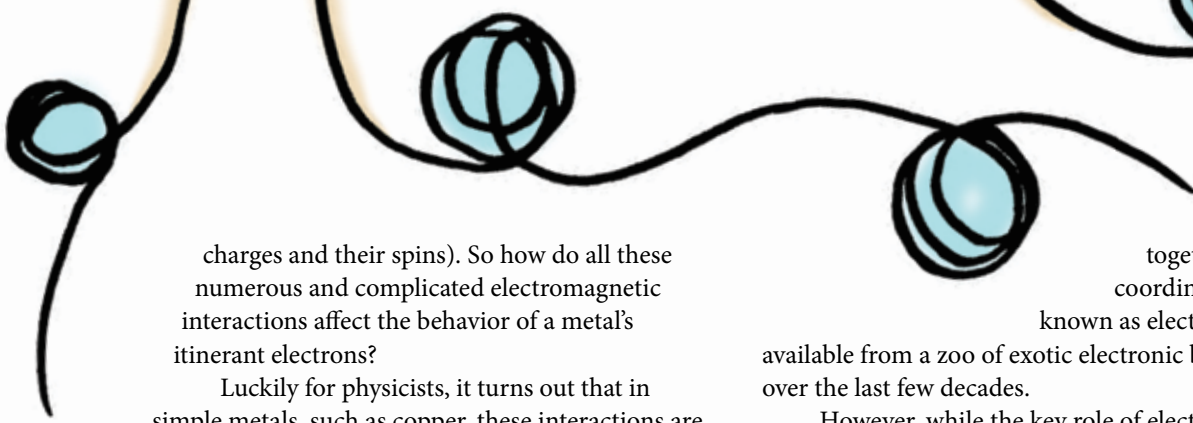
have more protons and electrons. Atoms of hydrogen have one of each, helium two, lithium three, and so on. Plutonium has 94. The protons (plus neutrons) pack into the nucleus, while the electrons successively fill available states, known as orbitals, outside the nucleus. Different orbitals, denoted with the letters *s*, *p*, *d*, and *f*, have different capacities, and it is the extent to which the outermost, or valence, orbitals are filled that determines an element's chemical properties and its position on the periodic table. Carbon atoms, for example, have four valence electrons and therefore four bonding sites, and correspondingly, they can form diamond, a four-sided crystal.

Against all odds, plutonium is the low-hanging fruit for studying electronic correlations.

This is basically the story of how the structure of the atom determines the behavior of the element. It's a great story, but it's not always complete. Rather, the structure of an atom can change in response to all the other atoms in a material, thereby changing the nature of the material itself. And a handful of material might contain trillions of trillions of atoms.

It is possible for neighboring atoms to reside far enough from one another that the valence electrons stay localized to their corresponding nuclei—roughly an ordered collection of isolated atoms. However, the atoms in a material can also lie so close to one another that the valence orbitals of neighboring atoms will overlap. In this latter case, it's often unclear which atom a particular valence electron should call home; therefore, some electrons are essentially free to wander through the material, making the material an electrical conductor (a metal). In the former case, where no electron is free to move away from its home atom, the material cannot conduct electricity and is called an insulator.

In the case of a conductor, however, additional complications arise. If each atom supplies, on average, one electron that's free to roam (or “itinerant”), then there will be as many itinerant electrons in the material as there are atoms. As they move through the material, they interact with one another (and with all the other electrons localized to their nuclei) via electrostatic repulsion (due to their negative charges) and via magnetic interactions (due to a combination of their negative



charges and their spins). So how do all these numerous and complicated electromagnetic interactions affect the behavior of a metal's itinerant electrons?

Luckily for physicists, it turns out that in simple metals, such as copper, these interactions are typically very weak and can be partially ignored. This is the basis for the Fermi-liquid theory, originally put forth in the 1950s, which is, in many ways, the standard model of solids. The theory describes the electrons in a solid as a collection of non-interacting “quasi-particles” that have the same properties as free electrons except for a slightly higher effective mass to account for their interactions with other electrons. Just as an Olympic sprinter would be slowed down by obstacles on the track, an itinerant electron is slowed down by other electrons in its path. And how much either one is slowed down can be approximated with additional mass instead of obstacles, as though the sprinter had packed on a few extra pounds over Thanksgiving and the electron had acquired a higher-than-textbook-value mass.

While this standard theory has been extremely successful for materials in which itinerant electrons undergo weak interactions, it fails to explain more complex materials. It fails spectacularly with plutonium.

One foot out the door

“The valence electrons of plutonium occupy a complicated no-man’s land between localized and itinerant configurations,” says Los Alamos’s Marc Janoschek. Janoschek is the collaboration leader for a groundbreaking new measurement of the dualistic nature of plutonium’s valence electrons, one that helps explain exactly how plutonium defies the standard Fermi-liquid theory. Yet this result applies not only to plutonium, but also to complex materials more generally, including many currently known materials that demonstrate unconventional forms of superconductivity and other electronic oddities.

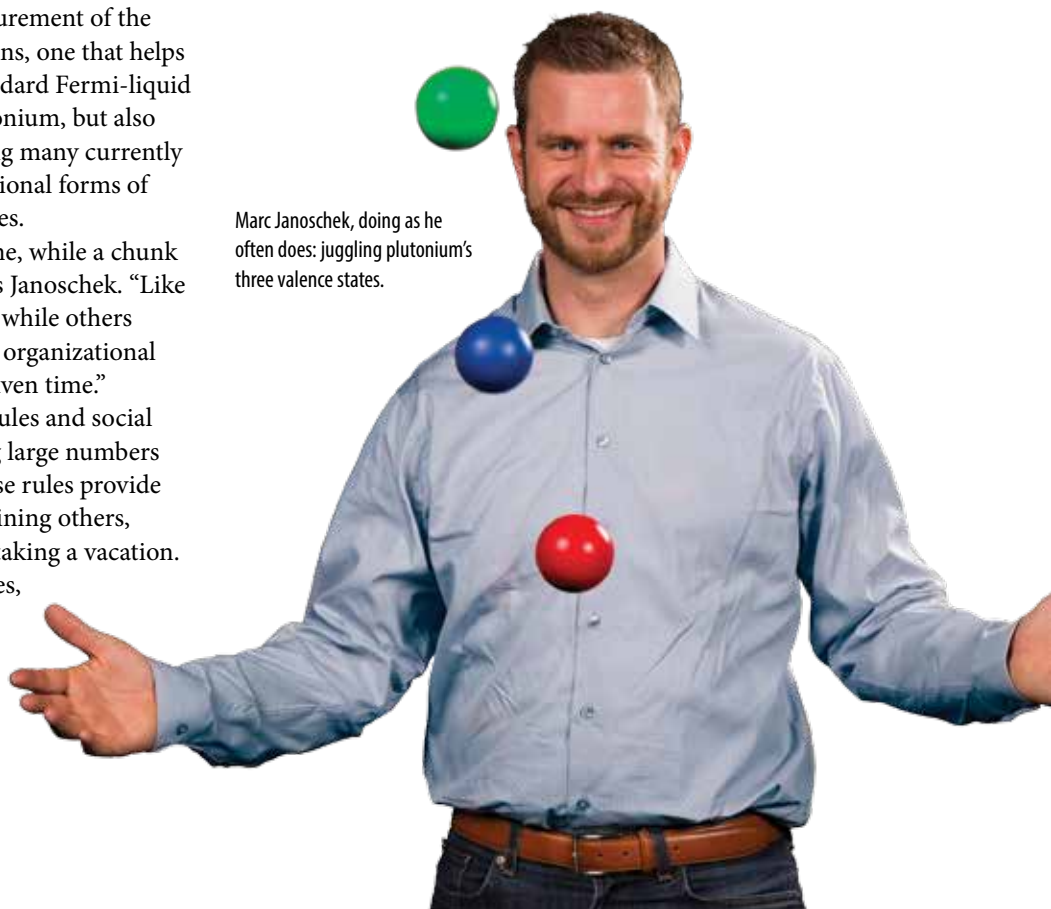
“Think of an individual atom like a home, while a chunk of metal is like an entire community,” explains Janoschek. “Like people, some electrons never leave the house, while others travel. And both communities respect certain organizational principles that affect who is traveling at any given time.”

Human communities are organized by rules and social structures that promote efficiency by allowing large numbers of individuals to contribute to the whole. These rules provide standardized reasons for leaving home and joining others, such as going to college, moving for a job, or taking a vacation. Electron communities, too, follow certain rules, in which multiple electrons (or in some cases, all of them) act in concert. Just as people are better off in a rule-abiding community, electrons save energy by acting

together. Evidence of such coordination among electrons, known as electronic correlations, is available from a zoo of exotic electronic behaviors discovered over the last few decades.

However, while the key role of electronic correlations in plutonium and other complex materials is well accepted among scientists, the exact rules that govern them—when valence electrons within the community are traveling versus staying home, or returning home, or visiting someone else’s home—are not well understood. With simpler metals, it is often sufficient to imagine that one or more valence electrons effectively make a choice to stay home or wander off and stick with that choice, localized or itinerant, forever. If the latter, then scientists treat them like free electrons and assign them a higher effective mass. But for a valence electron in plutonium, the stay-or-go decision is eternally in flux and dependent on all its neighbors, which are also in flux—a much more complicated situation.

What motivates material scientists and physicists like Janoschek to study strong electronic correlations despite the challenges is that they frequently lead to material properties that are critical for future applications. These include exotic varieties of superconductivity, conducting electricity resistance-free even at relatively high temperatures and making possible such technological boons as levitating trains, faster computers, inexpensive MRI systems, lossless transformers and power transmission lines, and other energy applications. They also include a property called colossal magnetoresistance, in which



Marc Janoschek, doing as he often does: juggling plutonium's three valence states.

(Lower frame) The atoms in the delta phase of plutonium are arranged in a face-centered cubic structure. This simple, well-defined crystal arrangement and the absence of other contaminating elements make plutonium suitable for neutron scattering experiments. Valence electrons bound to each atom interact strongly with the free-to-roam sea of conduction electrons that permeates the solid metal. These interactions cause fluctuations in the state of each atom, resulting in some atoms keeping all their electrons and others giving up either one or two. (Center frame) Each atom is constantly shifting among these three states and thus exists nominally in a blend of all three, time-averaging the different properties of each state—including different atomic sizes and intrinsic magnetism (upper frame). Fluctuations between states therefore imply fluctuations in magnetic properties, suggesting that plutonium's "missing" magnetism isn't exactly missing; it's just dynamic.

electrical conductivity changes drastically in the presence of a magnetic field, allowing for new spintronic and magnetic-sensing devices. Even the material properties of otherwise simple permanent magnets defy explanation without broadly coordinated electronic correlations.

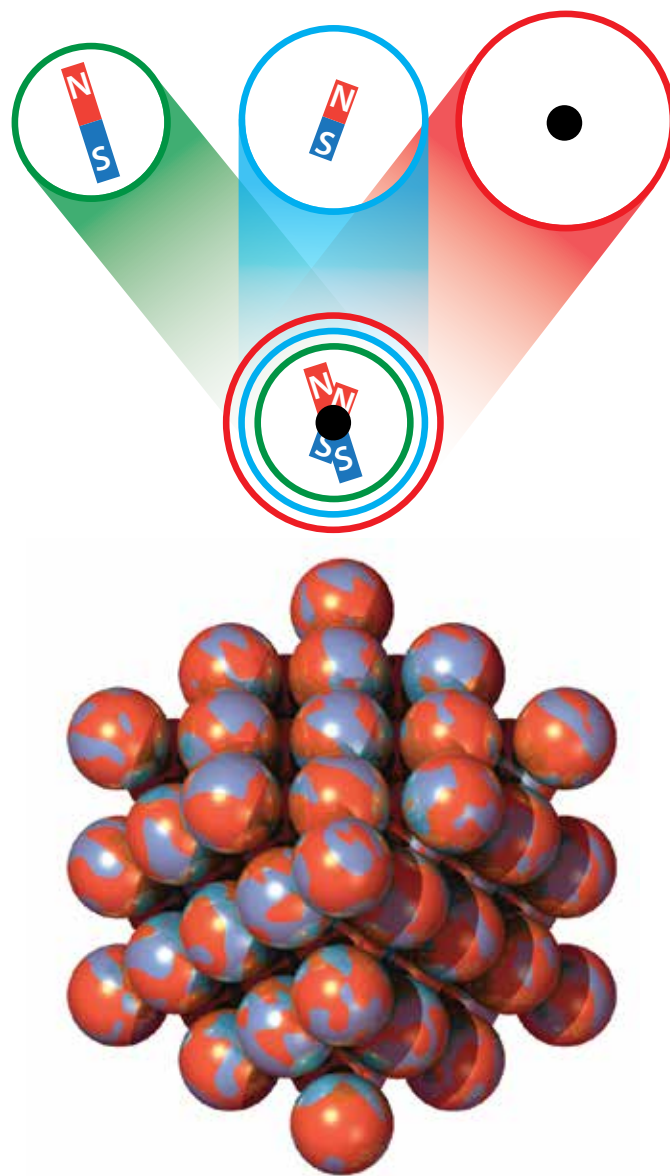
And then, of course, there's plutonium's missing magnetism. But when valence electrons are influenced by the entire electron community, their overall behavior changes, and the expectation of magnetism should change as well.

Not a home, a Kondo

In a way, plutonium defies periodic-table trends. Normally, for familiar metals with *d*-orbital valence electrons—like iron or gold or platinum—a higher atomic number means more protons and electrons, and the additional positively charged protons in the nucleus pull all negatively charged electrons inward to make the overall atom smaller. Conversely, for rare-earth metals with *4f* valence electrons, the additional protons have minimal effect on the overall size of the atom because the *4f* orbital resides close to the nucleus, and its additional electrons shield more distant electrons from the additional positive charges in the nucleus. But for actinide elements, which have *5f* valence electrons, the two effects compete: atoms get smaller with greater atomic number up to a point and then suddenly become larger and stay roughly the same size thereafter. (Care to guess which element occupies that transition point?)

The size and configuration of the atom affect material properties in two ways. First, they determine the extent to which an atom's outer electrons mingle with those from neighboring atoms, affecting how likely the electrons are to leave home and therefore affecting electrical conductivity. Second, if one or more electrons do leave home, that changes the configuration of those that remain, causing their spins and orbital motions to align differently, affecting magnetism. So roughly speaking, a localized *5f* valence electron participates in making the material magnetic, while an itinerant electron participates in making it metallic.

Earlier research revealed that plutonium's valence electrons live in an ever-shifting blend of three states: all valence electrons stay home, one leaves home, or, occasionally, two leave home. Theoretically, two of these states ought to be magnetic. But interestingly, in the third, valence electrons leave



home and have the possibility of interacting with magnetism-causing electrons (attached to their home atoms) in a way that nullifies the role of both electrons. This is known as the Kondo effect. It was first observed in normal metals laced with magnetic, transition-metal impurities (e.g., iron). There, conduction and magnetism-causing electrons pair up and cancel each other out at the location of each magnetic impurity.

But plutonium is its own impurity—two of its valence states, anyway—and that means the Kondo effect is constantly at work everywhere throughout the metal. Which electrons do what becomes a group decision because a magnetic cancellation in one spot can cause a state change in another, which encourages a conduction electron somewhere else to settle down, and so on. It's a never-ending interplay of electronic correlations that reaches every corner of the metal. Indeed, measurements of abnormally large electron contributions to the specific heat of plutonium lend support to this interpretation of Kondo-effect electron pairing with especially strong electronic correlations.

A research team from Rutgers University working in collaboration with Janoschek's Los Alamos colleague Jianxin Zhu developed calculations to examine this interpretation using an advanced methodology known as dynamical mean-field theory (DMFT). In the calculation, they treated the plutonium atoms as Kondo impurities. They found that magnetic atoms should come and go, pointing this way and that, never achieving a coherent alignment of the kind found inside genuinely magnetic materials.

"That means plutonium's missing magnetism isn't missing at all; it's dynamic," says Janoschek. "It moves and changes, driven by an ever-changing valence configuration. That makes it all but impossible to measure, which explains why all the measurements keep turning up no magnetism."

So there it is: the Kondo effect, electronic correlations, DMFT calculations, and dynamic magnetism—a nice, consistent story. And it's something scientists can apply to create all manner of advanced materials for the future, perhaps even leading to a whole new kind of electronics. But is any of it actually true? According to the pesky scientific method that every good scientist insists on using, an all-but-impossible measurement is the only way to find out.

Isotopes and allotropes

Janoschek decided to test the theory by bombarding a plutonium sample with neutrons to observe their deflection due to fleeting magnetic forces from the plutonium atoms. It's a straightforward experiment, one that's been tried before, but it can be riddled with confounding effects that must be painstakingly ferreted out.

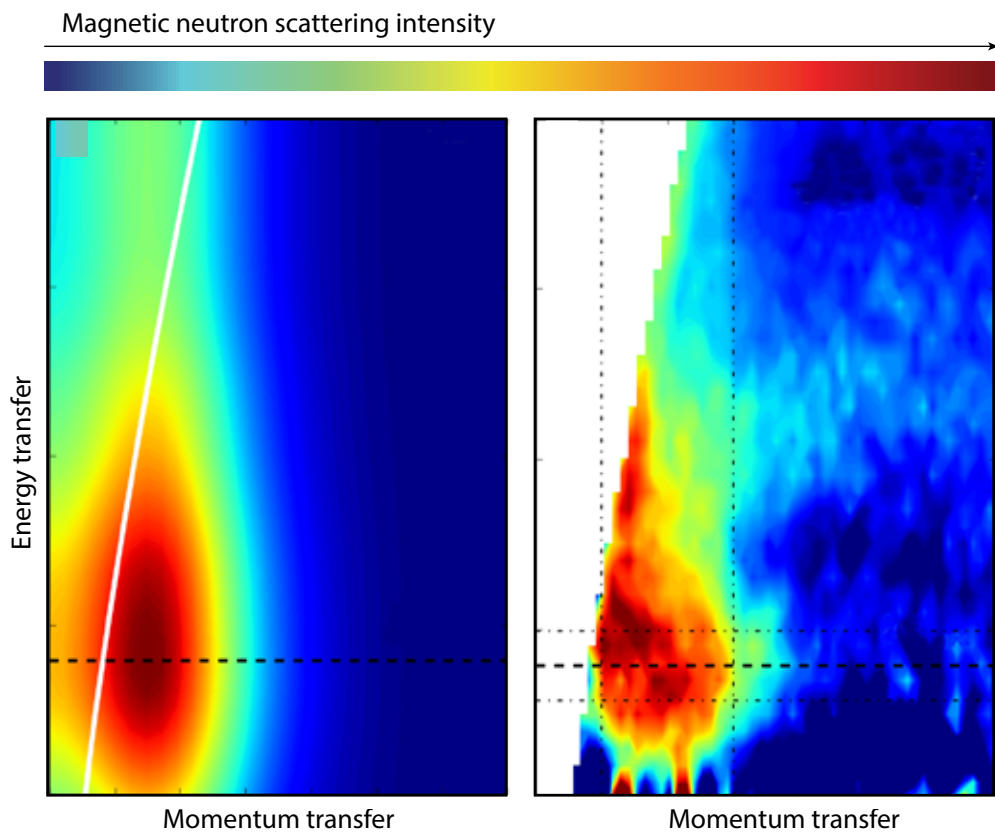
Because neutrons carry a magnetic dipole moment, a property that makes them act like tiny compass needles, they are sensitive to magnetic forces. That much is good for the experiment, but unfortunately, plutonium nuclei strongly absorb neutrons, which induce the nuclei to split in the process known as fission. Most of Janoschek's impinging neutrons would get lost in fission reactions before their magnetic deflection could be observed.

The standard theory to explain solids fails spectacularly with plutonium.

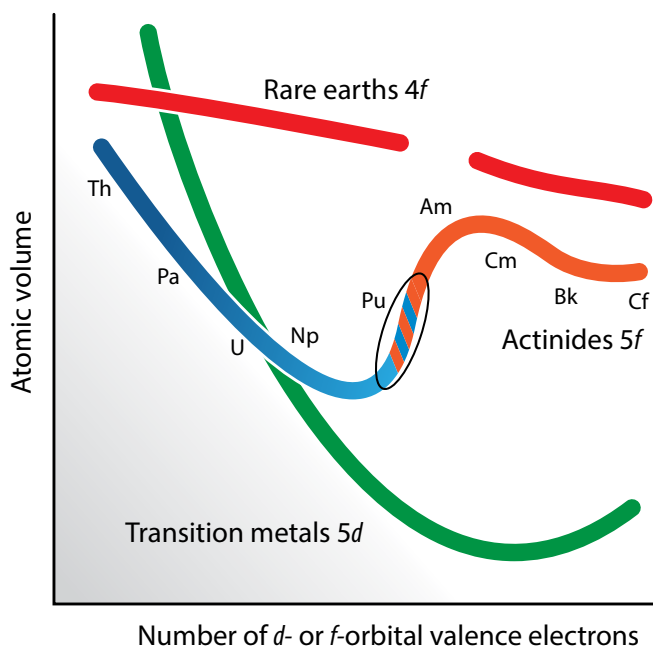
Help came from Los Alamos colleagues Eric Bauer, Jeremy Mitchell, Mike Ramos, and Scott Richmond, who knew how to prepare a sample made predominantly of plutonium-242, a rare, non-fissioning isotope with a far lower neutron-absorption rate than other isotopes. Bauer's research has been instrumental over the years in learning to work with plutonium-242. And because different isotopes of an element differ only in the number of uncharged neutrons in the nucleus, the behavior of their electrons is essentially identical.

After the neutron-absorption issue was solved, another confounding effect remained because, in addition to magnetic forces, neutrons are also deflected by nuclear interactions with protons and neutrons inside nuclei—from both the plutonium sample and its container. To tease out the magnetic effect,

Janoschek repeated the experiment on a sample of thorium with the same crystal structure as plutonium. Since the nuclear properties of both elements are well known, it was possible to compare them to isolate and then subtract the effects of nuclear deflection. Similarly, he was able to subtract the contribution from the sample container (which, for safety reasons, is doubly



Intensity map of magnetic fluctuations causing neutron scattering with respect to the momentum (x-axis) and energy (y-axis) transferred to the neutron. The left frame shows the expected experimental outcome from dynamical mean-field theory calculations; the right frame shows the actual neutron scattering results.



The sizes of different atoms on the periodic table generally follow predictable patterns. The actinide series of elements, however, with valence electrons in the 5f orbital, mimics the pattern for transition metals up to a point and then abruptly changes to mimic the pattern for magnetic rare-earth elements. Plutonium straddles the divide.

thick for plutonium samples) by scattering neutrons against an empty one. None of this is as simple or straightforward as it may sound, and with perseverance and attention to detail, he completed the experiment and the analysis.

It was quite the moment of triumph and, Janoschek admits, no small amount of surprise, when the experiment confirmed theoretical predictions: the most numerous deflected neutrons had energies characteristic of the transition between valence states, and the strength of the magnetism producing the deflections agreed with the DMFT calculations. The all-but-impossible experiment had been pulled off, and just like that, a five-decade-old scientific mystery was no more.

In addition, Janoschek's experiment provides a firm new basis for understanding plutonium's extraordinary allotropes. Similar to carbon with its well-known graphite and diamond allotropes, solid plutonium can be reconfigured as well. But it has an astonishing variety of configurations, and they differ so dramatically that a change from one to another, brought about by a change in temperature, can make the metal grow or shrink by an incredible 25 percent.

Yet even this extreme behavior can be understood naturally in terms of plutonium's extreme, ongoing fluctuations in electron localization and delocalization. When electrons come and go and reconfigure, that changes the atoms' sizes and the angles at which they form chemical bonds. Some configurations allow the atoms to pack together tightly, like packing a box with small cubes. Other configurations waste space, like trying to pack the box with

spheres instead, thereby expanding the volume. Combining plutonium's wildly shifting electron localization behavior with strong electron correlations throughout the material, it becomes easier to see how a temperature change might cause it to spontaneously reorganize in ways unmatched by other elements. And those reorganizations will naturally produce changes in material properties.

Strange bedfellows

It is perhaps a historical oddity that a new understanding of electronic correlations, both in terms of DMFT computations and neutron-scattering experiments, should come from plutonium. After all, this new understanding applies to a large number of materials, many of which, upon reengineering to take advantage of electronic correlations, are likely to offer greater societal rewards than plutonium. Yet the solution was discovered in plutonium, a nuclear weapons material available only to a small subset of scientists at a handful of high-security labs.

Plutonium, for all its complexity, happens to be the one material most suitable for this work. Against all odds, it is the low-hanging fruit for studying electronic correlations. It produces magnetic impurities and strong electronic correlations all by itself, without any other elements to complicate the analysis, and its delta-phase allotrope has a simple and regular cubic crystal structure. In these ways, plutonium makes both the theory and experiment accessible. And now that they are accessible, opportunities abound to develop electromagnetically ideal materials for novel magnetism- and superconductivity-based applications.

That isn't to say the benefits of this research reside exclusively outside the borders of the traditional plutonium-weapons world. One of Los Alamos's key charges is to develop the technology and expertise to protect the nation's nuclear weapons so that they remain safe and reliable over the decades. But aging plutonium—ravaged day by day by its own radioactivity—is even more perplexing than fresh plutonium, and keeping it under control is painstaking, diligent work. For those who do that work, there's tremendous potential to be found in the more comprehensive understanding of plutonium that Janoschek and his colleagues have now provided. For the wider electron-correlation research community, there's excitement and opportunity for advanced materials. And for everyone else, there can be an appreciation of progress—and perhaps a little relief. **LDRD**

—Craig Tyler

The Mold Rush





WE WERE WARNED. The rise of antibiotic resistance is not a surprise. In 1945, when Sir Alexander Fleming accepted the Nobel Prize for his discovery of penicillin, he suggested that society should be careful with antibiotics and that misuse would lead to resistant organisms. He was right, and throughout the last 70 years, he was not the only one to sound an alarm.

Society is now on the brink of losing the ability to fight dangerous infections. Bacteria have gained resistance to our arsenal of antibiotics and have shared their strategies with each other. The once-revered miracle drug penicillin that revolutionized medicine—a compound made by blue-green mold with the express purpose of fighting off its enemy bacteria—is now rarely used, and most of its derivatives are dropping out of commission one by one.

However, while negligent use may fuel resistance, the problem is intensified by the fact that very few new antibiotics have been approved in the last few decades. The high cost of research and clinical trials, coupled with the fact that resistance is a natural phenomenon that will inevitably render new drugs useless after some period of time, makes their development less profitable. In fact, many pharmaceutical companies have not researched new antibiotics since the 1990s.

While many warn of an antibiotic apocalypse, Los Alamos structural biologist Alex Koglin remains hopeful. His passion for understanding the structures of proteins and enzymes has led him to a novel approach for identifying new therapeutics. But that's not all. Using this technique, he and his team mined the genomes of thousands of organisms, and earlier this year they discovered two *completely new* antibiotics.

Miracle mold

As the story goes, the discovery of penicillin in 1928 was somewhat accidental when Fleming, an English bacteriologist, returned from vacation to find that a mold called *Penicillium notatum* had contaminated his petri dishes. Upon further study of the situation, he was surprised to find that the mold prevented the normal growth of his *Staphylococcus* bacterial culture.

Microorganisms (microbes), like all living things, must compete for food and space in their ecological niche. Fleming had stumbled upon one of their natural defenses: the mold was secreting a small molecule that could kill its enemy, the staph bacteria. Later work by Howard Florey and Ernst Chain (who shared the Nobel Prize with Fleming, but not the fame) further examined the small molecule they called penicillin and showed it could be isolated, produced, and used as a treatment against infections in humans. The resulting miracle drug was widely used during World War II for stopping infections from wounds and amputations and is credited with having saved thousands of soldiers' lives. Subsequently, penicillin was quickly marketed to the general public as a cure-all for everything from ear infections to gonorrhea.

After the discovery of penicillin, many other antibiotics were isolated from microbes for use in medicine, while others were developed synthetically by slightly altering the structure of existing antibiotics. For decades, new therapeutics were approved at a steady pace, but in the late 1980s and 90s, the numbers began to level off and then dropped dramatically over the last 15 years.

Why? Some argue that pharmaceutical companies have abandoned the search for antibiotics to focus efforts on more profitable therapies for chronic diseases such as cancer, heart disease, or diabetes—for which patients purchase drugs regularly, year after year. However, others argue that all the easy-to-

find antibiotics have already been found, and that developing new antibiotics that are effective against drug-resistant bacteria is a difficult task. Adjusting the chemical structure of an antibiotic to make a new one requires careful attention

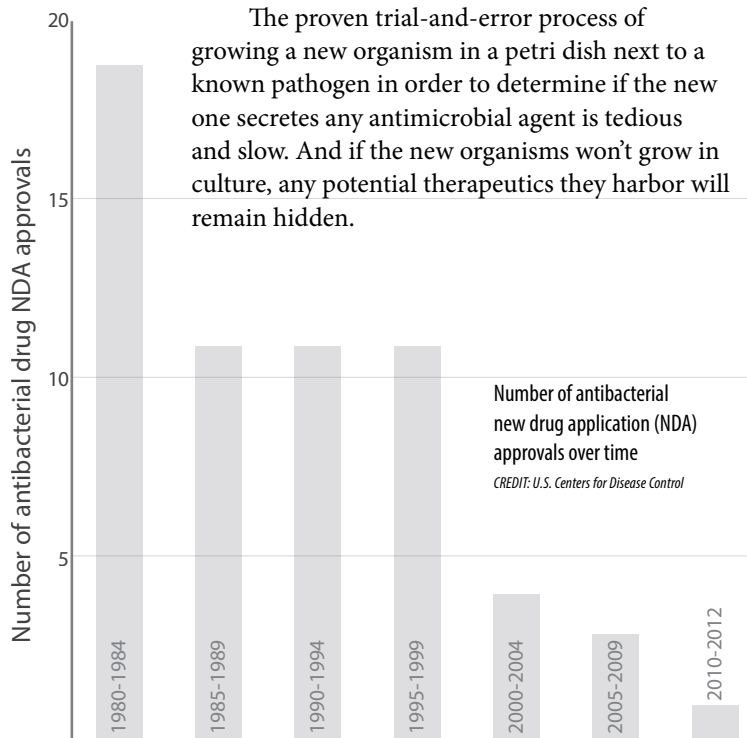


Antibiotics are small compounds made naturally by microorganisms for survival; some are made to kill other organisms that threaten their food supply or living space. (Left) The space between two different molds indicates that one is secreting a compound that inhibits the growth of the other. (Right) How this concept is tested in the laboratory: Small paper disks treated with antibiotics isolated from microorganisms are placed on a plate of bacteria. The area around the paper where no bacteria are growing shows that the antibiotics are working to kill the bacteria, as expected. However, a few antibiotics do not have clearance zones around them, indicating that the microbes are resistant to those particular drugs.

to ensure the new compound is not toxic and still works as desired. But since the resulting structure will be similar to existing drugs, it may also be more susceptible to already-developed bacterial resistance.

On the other hand, finding completely new drugs is also a challenge. There are billions of microorganisms out there in the world (in the soil, in the oceans, in our bodies) and likely all of them have developed defense mechanisms to fight each other. In order to take advantage of this plethora of potential drugs—not only antibiotic agents, but, to name a few, anti-inflammatory, anti-cancer, and anti-viral ones as well—these microbes must be studied in a lab. However, due to the fact that most of them require complex environments in which to grow, scientists have only discovered and cultivated a mere 1 percent of the planet's estimated microbial diversity.

The proven trial-and-error process of growing a new organism in a petri dish next to a known pathogen in order to determine if the new one secretes any antimicrobial agent is tedious and slow. And if the new organisms won't grow in culture, any potential therapeutics they harbor will remain hidden.



What would Darwin do?

“Nature had and still has endless evolutionary time to develop small bioactive molecules to kill bacteria,” says Koglin. “We have to accept that a potential solution for our current public health needs with multi-drug resistance is likely out there, but we have to change the way we look for it.”

Koglin's strategy begins with understanding how antibiotics are made by microbes. Antibiotics are small molecules often referred to as secondary metabolites because the cell produces them for a valuable purpose that does not include the primary functions of growth, development, or reproduction. Secondary metabolites might instead be molecules that help the organism adapt to its environment (such as binding to certain nutrients) or protect it by killing enemies.

Since defense molecules such as antibiotics are toxic, they could potentially hurt the host cell that makes them, so they are highly regulated. In order to do this, microbes make antibiotics using special enzyme complexes; one class of these enzymes is called nonribosomal peptide synthetases (NRPSs). This is in stark contrast to the way most other products are made by the cell.

Most cellular products are made by protein complexes called ribosomes following directions from the cell's genomic material (DNA): a transcript (made of RNA) of the directions is made and then translated by a ribosome into protein. Antibiotic compounds are different; they are not directly coded for in the genomic material at all. Instead, the genome contains instructions for the specific NRPS complex needed to make each antibiotic or other secondary metabolite. In other words, the genome encodes the tools, and the tools make the antibiotic (in or near the cell, somewhere the process can be regulated effectively to prevent damage to vital cellular components).

Threats such as food competitors, predatory organisms, or environmental changes (pH, temperature, food availability) trigger the production of NRPS complexes through the normal genome-transcription-translation process. Then NRPS

enzymatic components assemble in a highly specific order determined by the genetic sequence. Once assembled, the complexes begin producing metabolite compounds—in assembly-line fashion—to respond to the threat. Each enzyme has a specific operation. Step by step, some enzymes build the backbone of the molecule, while another enzyme might add a hydroxyl (OH) group, or a methyl (CH₃) group, or, as in the case of a recent discovery by Koglin's team, an aldehyde (CHO). The chemical structure of the metabolite compound produced at the end is based entirely on the order of the enzyme complex: each NRPS cluster has a specific order and therefore a specific product.

As a result, an organism keeps instructions for an entire toolbox of NRPS complexes within its genome. This requires tremendous effort by the microbe, and an individual organism might not always have the correct NRPS tools to respond to the present threat. However, as Koglin explains, bacteria function



In the 1940s and 50s, penicillin was marketed to the general public as a cure-all for everything from ear infections to gonorrhea—and it worked. Unfortunately, decades later, gonorrhea is making a comeback as some strains have gained resistance to multiple antibiotics. These resistant strains are already becoming a major problem in Australia, France, Japan, Norway, Sweden, and the United Kingdom.

CREDIT: NIH

Resistance Matters: Too Much of a Good Thing



Just as some microbes evolve the ability to produce antibiotics for self-defense, those microbes and others can also evolve resistance to the antibiotic. The more antibiotics are used in humans and animals, the more bacteria become resistant. In the United States today, antibiotic-resistant bacteria cause about two million serious infections and 23,000 deaths per year.



In Industrial Agriculture

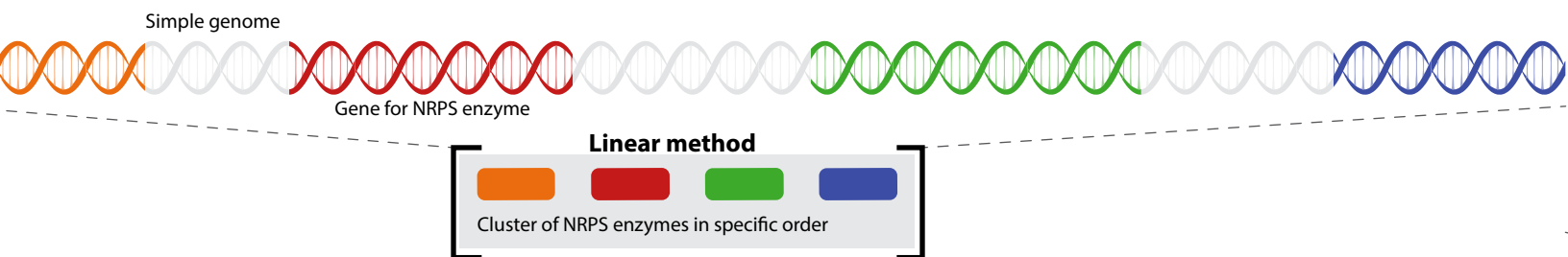
In the 1940s, as industrial agriculture began to expand, requiring animals to live in close quarters in large numbers, farmers began using antibiotics to keep them healthy. They quickly discovered that the drugs actually increased growth in the livestock and poultry, allowing the production of larger animals using less food, thus pushing down food costs. In 1977, the Food and Drug Administration (FDA) wrote a proposal to withdrawal approval for administering penicillin in animal feed, but it did not pass. Instead, meat production increased over the last few decades and a large portion of it has included the use of antibiotics such as tetracyclines, penicillin, streptomycin, and bacitracin, to name a few. In fact, the majority of the antibiotics sold in the United States (70 percent, according to the Pew Charitable Trust and PBS Frontline) are given to livestock.

This widespread use of antibiotics—especially for animals that are not sick—is creating large populations of resistant bacteria that can cause disease in humans. Furthermore, resistant bacteria from animals that have been fed antibiotics can spread if the animal manure is used to fertilize fields or is washed into waterways by rain. Although some agricultural representatives argue that the direct correlation of use in animals and disease in humans is difficult to prove, many studies have shown there is an impact. Likely with this in mind, the FDA issued a call in 2013 for the voluntary reduction of the use of antimicrobials for growth enhancement in livestock—followed by Tyson foods and McDonald's announcing earlier this year that they will begin to limit the use of antibiotics in their chickens.

In Medicine

According to the U.S. Centers for Disease Control, over half of the antibiotics prescribed for patients are inappropriate. This means that in many cases, a patient suffering from a viral infection will be given an antibiotic, which will not do anything to fight the infection. Instead, it will give any bacteria in the patient's body a week's worth of exposure to the drug, which can fuel resistance. In one study, only 10 percent of adults who had a sore throat actually had strep (a streptococcal bacterial infection that requires antibiotics); however, 60 percent of patients with sore throats were given antibiotics. Conversely, if a patient is correctly given antibiotics for a bacterial infection but does not finish the full prescribed course, there is an increased possibility that some bacteria will survive and may become resistant through the limited exposure.

Changing this situation requires educating both the public and the medical community. However, another improvement could come with advanced diagnostic tools. Doctors can test a patient with a sore throat to find out if it is indeed caused by streptococcal bacteria, but such tests cost time and money, and there are not reliable, affordable tests for all possible infections. Research and development of new, less-expensive diagnostic tools that can rapidly screen for multiple diseases at a time could give doctors the information they need to treat patients more effectively and responsibly.



together as a species, and the survival of the individual is not the priority. Through a process called horizontal gene transfer, bacteria can exchange genes for their NRPS complexes to other bacteria to help their colony survive. And the genes are reorganized in the recipient organism's genome to create novel clusters that will produce new compounds. Indeed, this serves as a good example of survival of the fittest because if the compounds created don't work to eliminate the threat, the bacteria are more likely to die. However, if at least one bacterium in the colony creates a compound that allows it to survive, it may spawn a new colony equipped with its successful NRPS tools.

Because the antibiotic produced can be highly toxic to the organism that made it, that organism must sometimes evolve resistance to its own defense mechanisms. This resistance is also transferred to others in the colony, which is helpful so long as the resistance doesn't get transferred to the organism the antibiotic is supposed to kill, in which case it is no longer useful. So alternatively, a microorganism might defend itself against its own dangerous metabolites in other ways. Koglin and his recent postdoc Matthais Strieker (who now holds a faculty position at the University of Braunschweig in Germany) actually discovered examples of secondary metabolites that are so toxic they cannot be entirely produced inside the host cell. Rather, only precursor molecules are made in the cell and then immediately exported so their biosynthesis can be completed outside of the host.

Targeting the toolbox

Not surprisingly, many researchers in academia and industry have focused on examining the NRPS toolbox to find new antibiotics. Fascinated by the structures of NRPS clusters and their ability to create different compounds based only on the order of their components, Koglin and Strieker began to

seek an understanding of the driving forces for NRPS enzyme cluster assembly. Their hope was that if they could understand the clusters better, they might discover how to find novel ones that make novel antibiotic compounds.

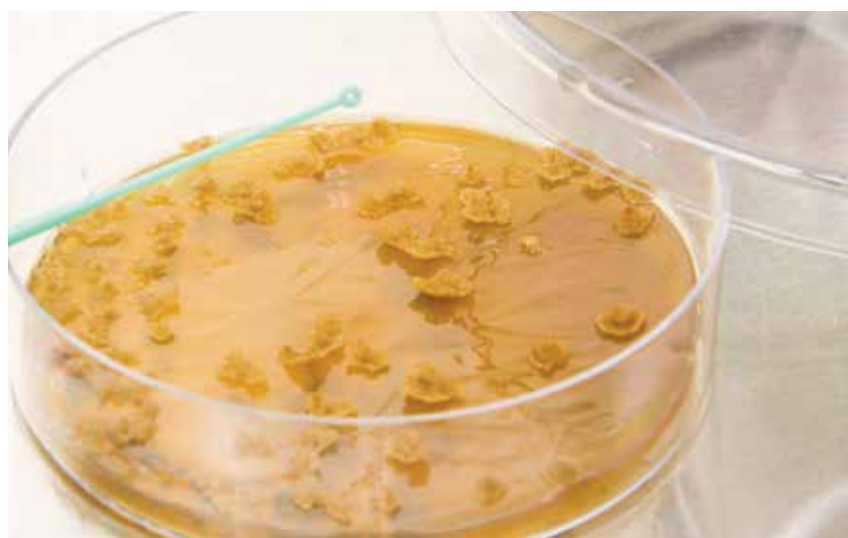
To do this they needed to determine which NRPS assembly lines exist in which organisms, so Koglin and Strieker turned to their Los Alamos colleagues' expertise in genomics, bioinformatics, database development, and microbiology to screen the microbial, fungal, and plant kingdoms. Those colleagues included bioinformatics scientists Jean Challacombe and Scott Hennelly, the Bioscience Division genome team, and microbiologist Chris Yeager.

Nature had and still has endless evolutionary time to develop small bioactive molecules to kill bacteria.

Over the last decade, genome sequencing has made significant advances, in particular with the invention of metagenomics—a method that enables entire communities of microorganisms to be sequenced at once without having to culture them individually. The resulting explosion of widely available genome-sequence data ensures an ample supply of newly discovered organisms that can be mined for novel compounds.

With metagenomic sequence data and expert collaborators at hand, Koglin and Strieker set out to study the clusters. Koglin explains that many people look at the genes for NRPS enzymes linearly, but that he and Strieker wanted to find a cluster that was truly different, with the hope that it might be less susceptible to resistance. So they needed a new approach.

Streptoporphyrin roseum and *Catenulipora acidiphila*: two organisms the Los Alamos team is investigating for new drug candidates.





Complex genomes

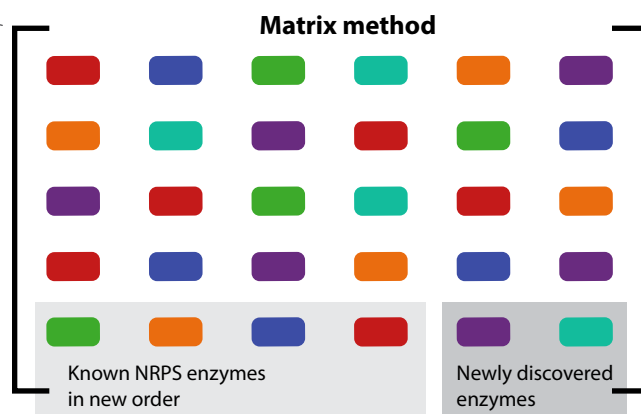
Nonribosomal peptide synthetases (NRPSs) are clusters of enzymes that make antibiotic compounds. In an effort to find new antibiotics, scientists search the genomes of new microorganisms for the genes that encode NRPS enzymes. It is relatively easy to find the genes if they always exist in the same linear order in the genome; however, in complex organisms that organize their DNA on multiple chromosomes, the genes might be spread out and more difficult to identify. In an effort to find NRPS clusters that are truly different, with the hope that they might be less susceptible to resistance, Los Alamos scientists developed a matrix method to find the genes for those NRPS enzymes wherever they might be in the genomic data—even if they are not found together. The result: they were able to discover known enzymes in new orders as well as new enzymes that together produce a completely new class of antibiotic compounds.

First, they examined the known functions of each of the enzymes necessary to create an antibiotic-type, or bioactive, molecule. With this information, they developed an algorithm to find the genes for NRPS enzymes wherever they might be in the genomic data—even if they are not found together. For instance, in a complex organism like a plant that has its genes organized on chromosomes, the NRPS genes for one cluster could be found spread out on different chromosomes. And once they found the pieces of a cluster, they began to examine which other genes were nearby that might be new and potentially involved in NRPS synthesis.

It's kind of like looking for all the words in a sentence, but not requiring that they be in the right grammatical order—just whether certain words are there, within certain proximity parameters. This led to a matrix-type approach that allowed Koglin and Strieker to screen vast amounts of data—genomes from thousands of unknown microbes—to determine which organisms have the right tools encoded in their genomes for producing bioactive molecules that have potential as new antibiotics.

To accelerate the screening process, Challacombe has been developing a relational database to enable parallel searches and alignments. “The goal is to put all the powerful tools in one place to do the analysis,” she says. “That way, if you find one NRPS cluster in one organism, you can determine if it looks the same in another.”

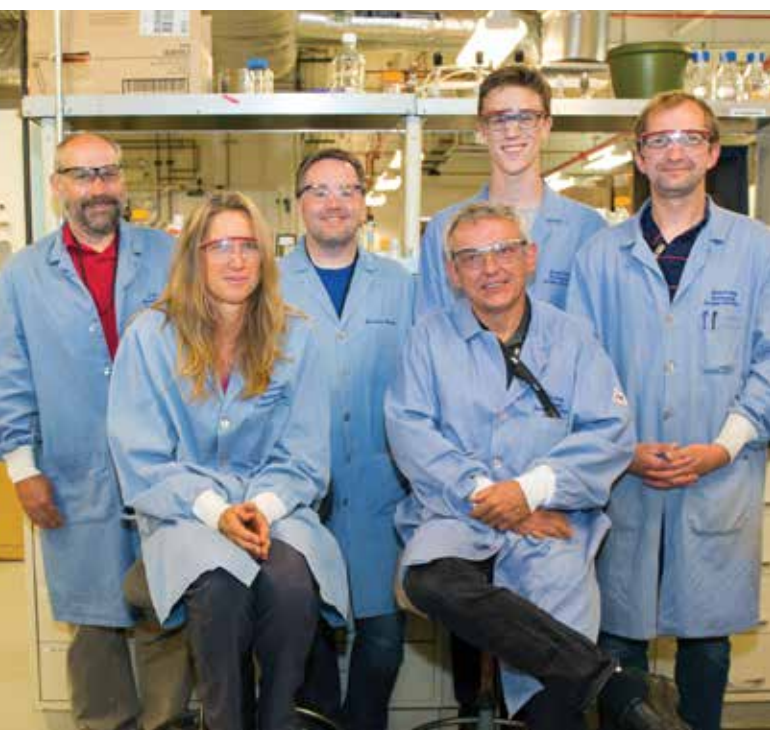
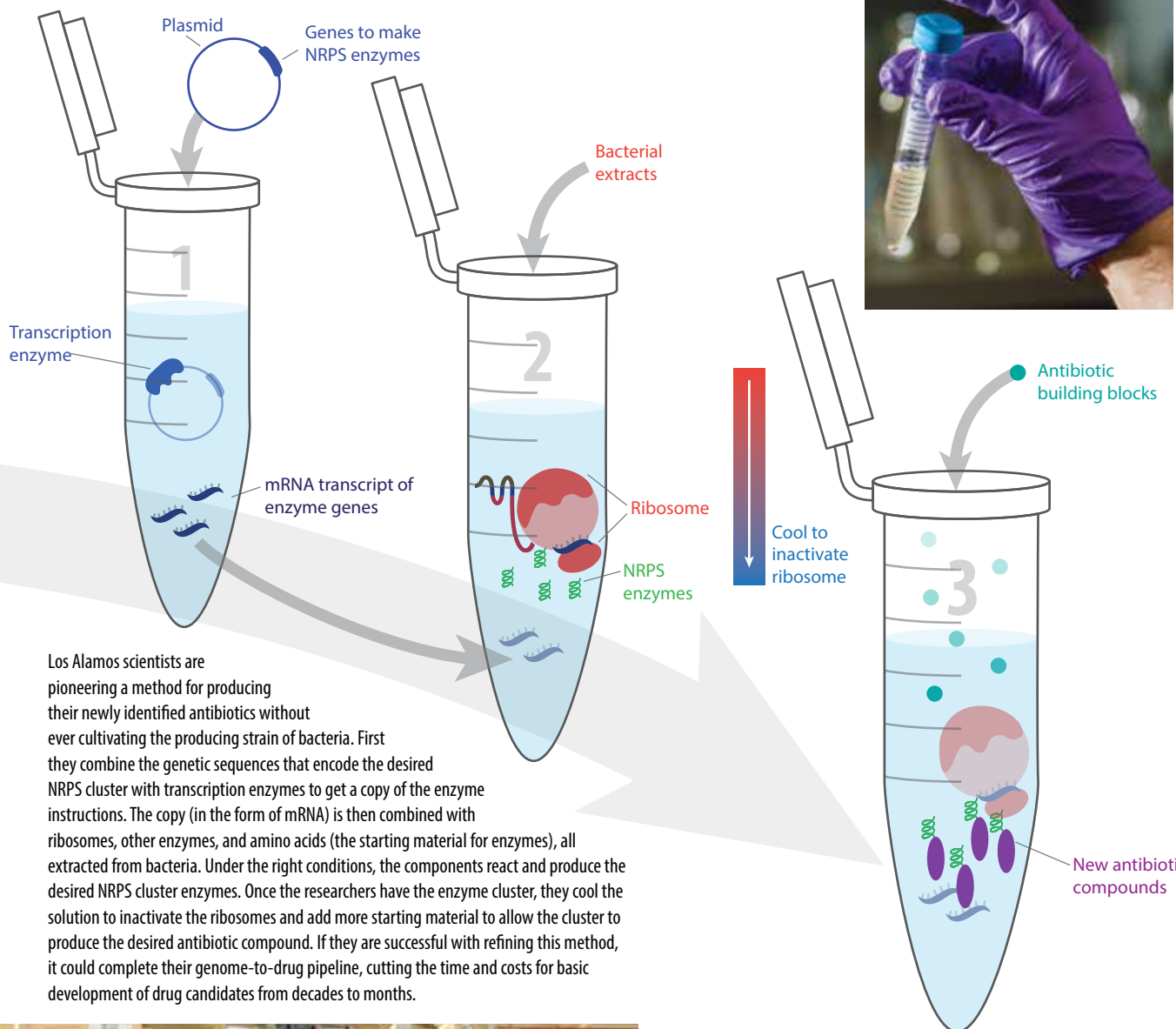
The team used this matrix approach to screen 30,000 clusters of enzymes in over 4,000 plant, fungal, and bacterial genomes. From this, it was able to identify 16,000 clusters that would make something completely new. The team further narrowed its results by searching for very specific criteria, such as certain amino acids or side chains, the ability to integrate into a membrane, the activation of key enzymes, etc. In the end, the researchers found five new bioactive compounds they predicted could be useful as antibiotics.



Among the NRPS clusters that produced these five compounds, two clusters caught the team's attention by the fact that they produced practically identical compounds but had evolved independent biosynthetic pathways to do so in completely different organisms: one, an anaerobic hyperthermophile called *Clostridium thermocellum*, and the other, a cold-lake predatory bacterium called *Herpetosiphon aurantiacus*.

Along with Los Alamos chemist Jurgen Schmidt, the team began to further examine the enzyme clusters in these two organisms and the compounds the clusters produced. Although the scientists still do not fully understand the mechanisms of the clusters or their order, they sought to elucidate the chemical structures of the metabolite products using stable-isotope labeling (adding a heavier carbon-13 atom instead of a normal carbon-12 to allow tracking), mass spectrometry, nuclear magnetic resonance, x-ray crystallography, and neutron scattering. (“The convenience of having this comprehensive suite of capabilities at our fingertips—as well as genomic sequencing and computation—is a unique advantage for scientists at Los Alamos,” says Schmidt.) In the end, they isolated and named an antibiotic compound called thermocellomycin from *C. thermocellum* and one called aurantiamycin from *H. aurantiacus*.

Once the new compounds were isolated and characterized, the team could test thermocellomycin and aurantiamycin for antimicrobial activity. The results have been impressive. Both new compounds were shown to inhibit the growth of 13 pathogen species, encompassing over 20 strains. This list included known, highly problematic resistant strains such as MRSA (methicillin-resistant *Staphylococcus aureus*, which causes deadly skin infections) and *Clostridium difficile*



Left to right: Scott Hennelly, Jean Challacombe (seated), Michael Humbert, Jurgen Schmidt (seated), John M. Gordon, and Alex Koglin

(which causes a life-threatening gastrointestinal disease), as well as *Bacillus anthracis* (which causes anthrax) and *Yersinia pestis* (which causes the plague).

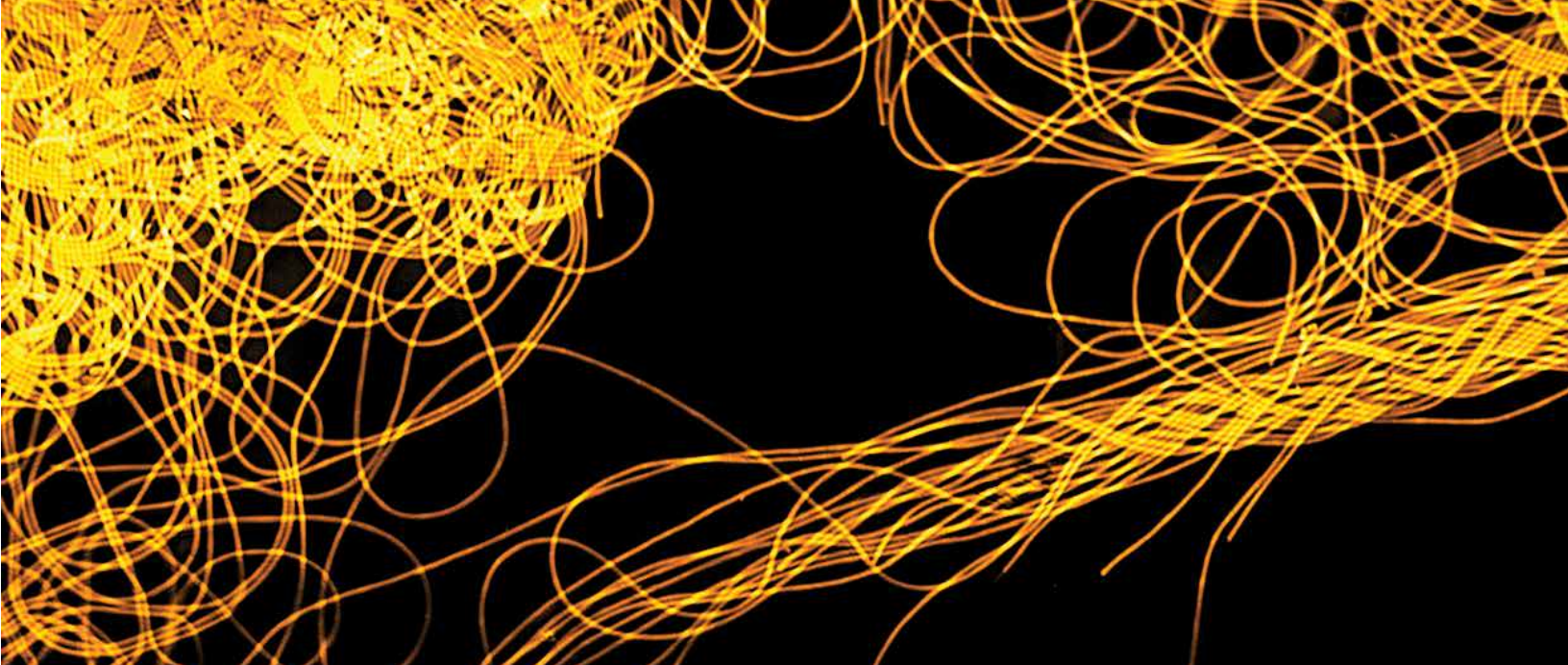
“What we’ve found here is a completely new class of antibiotics,” says Koglin.

The road to the medicine cabinet

In the 1940s, when society began to produce penicillin on a large scale, the challenge was to grow enough *Penicillium notatum* mold in containment so that the drugs could be siphoned off. Today, large-scale production of antibiotics generally still relies on growing microbes.

If the new Los Alamos drug candidates thermocellomycin and aurantiamycin are ever to be approved for widespread use, they will have to be produced *en masse* as well. However, the Los Alamos team has not yet been able to culture these organisms in large quantities, nor has it been successful in producing thermocellomycin and aurantiamycin using alternative host organisms.

To address this aspect of the challenge, the team is developing a method to produce the newly identified antibiotics without cultivating the producing strain of bacteria.



Los Alamos scientists recently isolated the new antibiotic aurantiamycin from this bacterium, *Herpetosiphon aurantiacus* (shown here in a photo taken with a specialized type of optical microscope). Aurantiamycin has already demonstrated effectiveness against 13 pathogen species, including highly problematic resistant strains such as methicillin-resistant *Staphylococcus aureus* and *Clostridium difficile*, and is currently being tested for toxicity in animals before consideration by the Food and Drug Administration.

CREDIT: Marine Biological Laboratory/Irina Arkhipova and Michael Shribak

The method relies on combining all the necessary components (the genetic sequences that encode the NRPS cluster, transcription enzymes, and ribosomes) in a vial at the right temperature and pH so that the components react to produce the desired NRPS cluster. Once the team has the enzyme cluster, it should be able to add amino acid building blocks so that the NRPS cluster can produce the antibiotic compound—all without the need for a live host organism.

“It would be a tremendous shortcut not to have to grow the organism,” says Michael Humbert, a guest scientist working with the Los Alamos team. Humbert, who is a specialist when it comes to host-free biosynthesis, explains that the ribosomes have to be especially stable in order to survive the lengthy process of creating large amounts of enzyme clusters. The team had been using *E. coli* enzymes, but they are not holding up to the stress of the production line, so it is now trying ribosomes from different thermophilic (heat-loving) organisms because of their increased stability.

What we’ve found here is a completely new class of antibiotics.

In the meantime, while the Los Alamos team is working on improving its production method, the United States Army Medical Research Institute of Infectious Diseases is busy testing thermocellomycin and aurantiamycin for toxicity in animals and doing further analysis of the drugs’ effectiveness against biothreat strains. If all goes well, the new antibiotics could be headed for Investigative New Drug Approval, a critical requirement preceding clinical trials as part of the process to gain Food and Drug Administration approval.

However, the real advancement here is that if Koglin and his collaborators can successfully produce thermocellomycin

and aurantiamycin in the laboratory without the need for growing the organisms, then they will have developed a complete genome-to-drug pipeline, cutting the time for basic development of drug candidates from decades to months.

In contrast to Fleming’s serendipitous discovery of penicillin, the Los Alamos scientists demonstrated a new strategy to selectively screen the microbial kingdom for the tools needed to create antibiotics. This strategy enabled their discovery of two new potential drugs, thermocellomycin and aurantiamycin, but it also showed how a targeted analysis of the NRPS toolbox could be used to find therapeutics. This approach could be used again and again, so as bacteria develop resistance to new drugs, scientists will have a reliable way to stay ahead of the game by continually discovering more new compounds. Moreover, the team’s efforts to produce new antibiotic compounds without ever cultivating an organism stand to greatly accelerate therapeutics production in general. Together, these achievements have the potential to revolutionize drug development. And there is nothing accidental about that. **LDRD**

—Rebecca McDonald

More therapeutics research at Los Alamos

- **International workshop on understanding drug resistance**
www.cnls.lanl.gov/drugresistance
- **Antibiotic-resistant tuberculosis’s strategy revealed**
www.lanl.gov/discover/publications/1663/2015-january/fighting-tuberculosis-in-the-21st-century.php
- **Analysis of the molecular mechanisms that underlie bacterial persistence**
cdn.intechopen.com/pdfs-wm/47762.pdf
- **Advanced diagnostics could improve antibiotic usage**
www.lanl.gov/discover/news-release-archive/2013/April/04.19-advancing-the-art-of-tuberculosis-detection.php

Getting to Know Our Neighbors

Los Alamos continues its legacy of space exploration by helping to build a better rover.

FOR HUNDREDS OF YEARS earthlings were the kind of solar-system neighbors who stayed home, peeking through their curtains and listening at their doors. But in 1997 that changed, and humans became the kind who stride across the lawn and ring the bell. Or, more aptly, the kind who thrill in sending a drone-mounted GoPro to scope out neighbors' yards and peer through their windows.

Humanity's previous exploration of Mars consisted of distant or limited observations, first by way of earthbound telescopes, then spacecraft fly-bys, followed by relatively primitive orbiters, and finally sessile landers. In 1997, the rover *Sojourner* made the first tracks on the Red Planet, roaming for about three Earth-months before contact was lost. (That may seem like a short period, but it was more than 10 times the intended mission duration.) In 2004, twin rovers, *Spirit* and *Opportunity*, with improved instrumentation and longer life expectancy, began their missions on Mars—11 years later *Opportunity* is still going, having survived more than 45 times over its original mission duration of three Earth-months. *Curiosity*, the latest rover to land on the fourth rock from the Sun, began its exploration in 2012 as part of NASA's Mars Science Laboratory project and is still trundling about, investigating Martian climate and geology.

A key instrument riding on *Curiosity* is the Los Alamos-designed ChemCam, which rapidly analyzes surface materials via a technique also developed largely at Los Alamos, known as laser-induced breakdown spectroscopy, or LIBS. Basically it zaps a rock with a laser then analyzes the colors that make up the resulting flash, from which it can infer the chemical composition of the rock. That is the chemistry, or Chem, in ChemCam; the Cam is a remote micro-imager that provides high-resolution black-and-white images of the sampled targets. In its first few years of operation ChemCam has examined thousands of samples in the interest of determining the presence or history of water on Mars and the suitability of the surface for eventual human explorers.

Sometime in 2020, an as-yet unnamed rover bearing a next-generation, souped-up ChemCam, called SuperCam, will join *Opportunity* and *Curiosity* on Mars's dusty surface. What makes SuperCam super lies in both the Chem and the Cam. First, while ChemCam produces black-and-white images, SuperCam's images will be in high-resolution color. Second, SuperCam will combine LIBS with Raman and infrared spectroscopy.



Los Alamos scientists helped to develop the instrument suite aboard the Mars orbiter *Odyssey* that was largely credited with the discovery of water in the form of ice beneath the planet's surface.



There are presently six active spacecraft orbiting around or driving on Mars.



This year's high school graduates have never known a world in which there were no robotic vehicles cruising around on Mars.

The time it takes...

1	to grow 3 inches of hair	180 days
2	to travel to and land on Mars	254 days
	for a human baby to develop to term	280 days
3	for one Earth-year	365 days

A day on Mars lasts
39 minutes
longer than a day on Earth.



A compound image provided by ChemCam's high-resolution camera shows a series of 1.4-millimeter-wide pits in the Martian surface soil formed by the instrument's LIBS laser from a distance of 3 meters.

Credit: ChemCam/LANL/IRAP/CNES

Whereas LIBS reveals the elemental composition of a rock, that is, whether it is made of silicon, iron, or carbon, Raman and infrared spectroscopies reveal the mineral make-up of the rock, for example, whether it is feldspar, quartz, or olivine. Raman spectroscopy is based on light scattering and requires a different color, lower-energy laser than LIBS, so instead of a bright flash it produces a soft glow. Cleverly, the LIBS laser is being engineered so that it can switch modes and produce the beam needed for Raman spectroscopy too, helping to reduce the weight and complexity of the instrument. The infrared spectrometer, which observes the rocks in a much longer wavelength range than what human eyes see, will provide mineralogy data that complement the Raman data.

SuperCam's instruments will all rely on a calibration target assembly. These are small samples of rocks, a library of sorts, which are mounted on the back of the rover within sight of the laser. The identity and composition of each sample is known so an instrument can measure the known samples to calibrate itself before collecting readings from unknown materials. Some of the calibration targets occur naturally on Earth—like the igneous feldspar. Others, though, are mimics of Mars rocks created from earth materials based on what SuperCam's designers know so far about Martian geology.

"SuperCam is a primary science tool as well as a reconnaissance tool for other instruments," says Roger Wiens, Los Alamos planetary scientist and SuperCam project leader. In addition to the LIBS, Raman, and infrared analyses, the data that ChemCam and soon SuperCam gather can identify which samples ought to be examined by some of the other instruments in the rover's payload. One of these other instruments, new for the 2020 rover, is called SHERLOC (Scanning Habitable Environments with Raman and Luminescence for

Organics and Chemicals). It is a tool for detection of organic matter and mineralogical analysis that uses an ultraviolet laser and relies on a Los Alamos-designed-and-built detector.

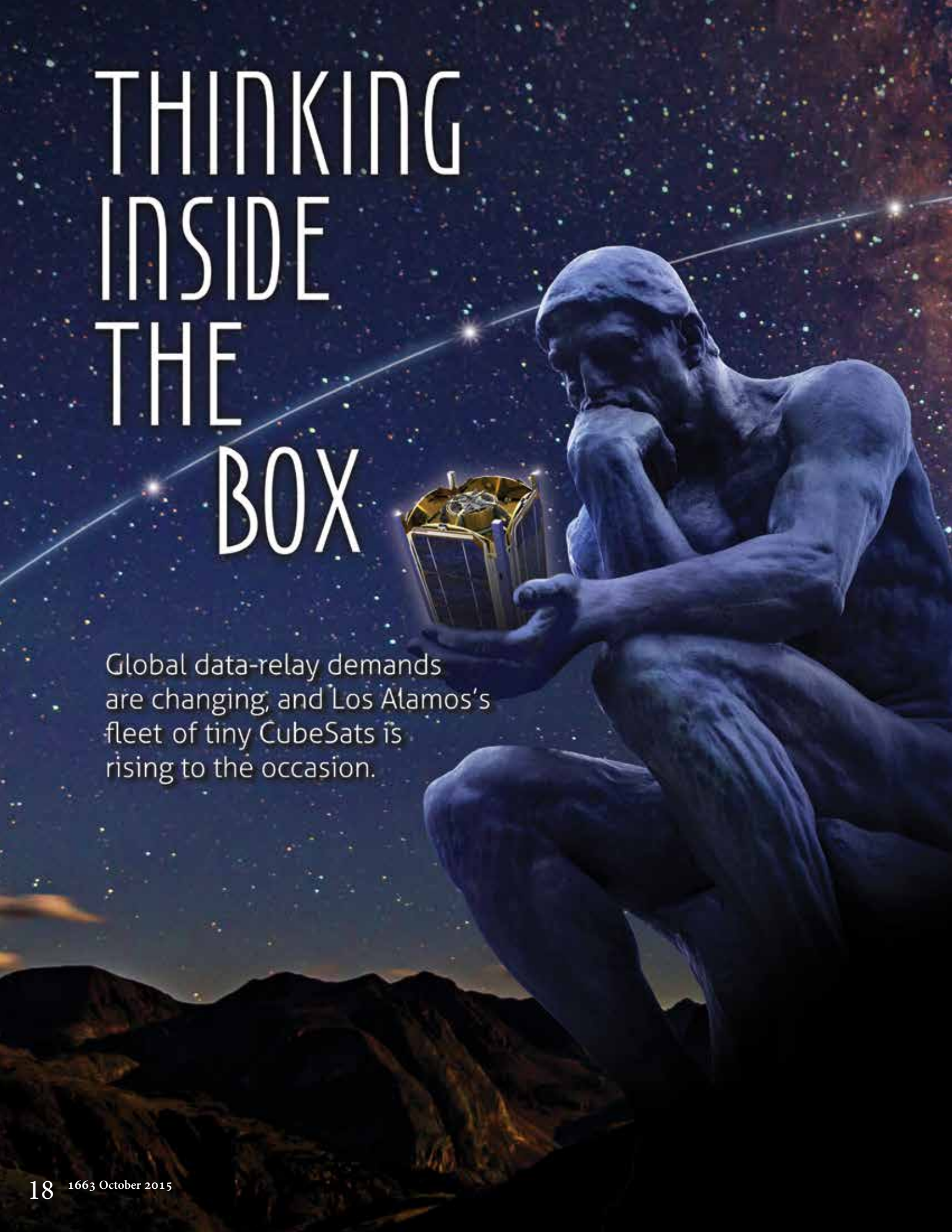
Turning momentarily to our other next-door neighbor, simulation experiments at Los Alamos have also proven the viability of a SuperCam-like instrument on a Venus lander. Whereas Mars is farther from the sun than Earth, and therefore cooler, Venus is closer to the Sun and hellishly hot. At 860°F and 90 times Earth's atmospheric pressure, the surface of Venus makes the inside of a pressure cooker look downright balmy. So the instrument on Venus would have to operate from within a protective pod, shooting its laser through a transparent window, similar in concept to a deep-ocean exploration vessel. Los Alamos ChemCam co-investigator Sam Clegg tested a SuperCam prototype under two sets of Venus-like conditions and showed that, while the instrument would necessarily be short-lived (it would melt after a few hours), it was capable of rapid operation in that time frame and could therefore prove useful. Although the United States has not yet landed a spacecraft on Venus (in 1970, Venera 7, a Soviet lander, was the first), NASA is continually exploring the idea of a future Venus lander. Clegg and Wiens have shown that a SuperCam-like instrument would be invaluable for helping scientists understand how Venus got so hot and how its atmosphere got so thick.

But for now their main focus is on being ready for Mars in 2020. They've proved the science and are busy building prototypes. Making everything smaller and more rugged is the key. Every component has to survive the vibration of launch and the impact of the explosives used during landing, which is tantamount to hitting the thing it's mounted on with a big hammer. Once there, it all has to function flawlessly in the extreme Martian landscape for as long as possible. So there is an incredible amount of engineering, testing, and perfecting to be done. Five more years may seem hardly enough time, but the SuperCam team and SuperCam itself will be ready.

Searching our planetary neighbor's yard for signs of ancient life is part of the Mars 2020 rover's mission. And because we've let ourselves in, and it appears that no one is home, exploring it as possible new real estate for humanity is the biggest thrill of all. **LORD**

—Eleanor Hutterer

THINKING INSIDE THE BOX

A composite image featuring the Statue of the Thinker, a bronze sculpture of a man in deep thought, holding a small, gold-colored satellite in his outstretched hand. The background is a deep blue night sky filled with stars and a bright, curved line of light, possibly a comet or a satellite trail. The bottom of the image shows a dark, rugged landscape with mountains under a twilight sky.

Global data-relay demands are changing, and Los Alamos's fleet of tiny CubeSats is rising to the occasion.



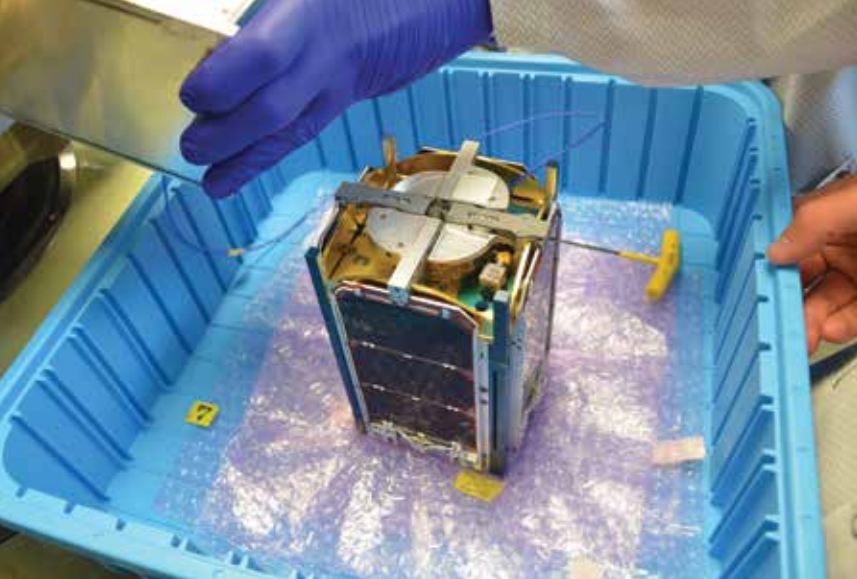
BARRELING THROUGH THE VACUUM OF SPACE at over 17,000 miles per hour, Earth's reflection glinting off its solar panels, the satellite is fiercely efficient and mission driven. It has hard edges and cold surfaces. It is brand new and state-of-the-art. It is an engineering masterpiece. And it's roughly the size of an electric pencil sharpener.

Satellites are generally thought of as hulking beasts of instrumentation. They are billion-dollar machines capable of gathering and relaying huge amounts of data to and from almost any point on Earth. The first man-made satellite to orbit planet Earth was Sputnik I, launched by Russia in 1957. The first U.S. satellite, Explorer I, went up about four months later. Since then, thousands of man-made satellites have gone into space and many remain there, dutifully reporting back to Earth or else dead and dark.

Building satellites was always a long and expensive process—large satellites like those that serve global positioning systems can take a decade to complete and cost hundreds of millions of dollars (the biggest satellites can run well over a billion dollars). Their operation, too, is highly specialized and extremely expensive, so historically, space has belonged to the very few groups who had the time, money, training, and perhaps importance to justify the enormous costs. Among those privileged few, Los Alamos has been involved in numerous U.S. satellite projects, almost since the beginning. Starting in the early 1960s with the Vela watchdog satellites following the limited nuclear test ban treaty, many of today's key satellites, such as NASA's Swift satellite (a space observatory dedicated to the study of gamma-ray bursts and the concomitant birth of black holes), carry Los Alamos-designed and Los Alamos-built hardware. Leveraging decades of experience and Department of Energy investment, Los Alamos is now leading the way in a different direction, with some of the smallest, most affordable satellites ever sent into space.

Thousands of man-made
satellites remain in space,
dutifully reporting back
or else drifting dead and dark.

When tiny satellites, called CubeSats (referring to the shape of the original model's stowed configuration, which was a cube measuring 10 centimeters on each side) were first invented in the late 1990s, they were seen as cheap, cute, and novel. They brought space within reach of everyone. Typically something that a college or graduate class might build together, with a modest budget over the course of a semester, a CubeSat could hitch a ride into space without much ado on a rocket primarily dedicated to larger, flashier cargo. But it could never be a contender for serious science. Or could it?



CubeSats are tiny, minimalist satellites, designed for very particular missions. The original was a cube measuring 10 centimeters on a side, defining the 1.0 U size. (Left) The Los Alamos CubeSats are taller at 1.5 U. (Second from left) Prometheus mechanical engineer Dan Seitz fine tunes a CubeSat in the lab, painstakingly perfecting every detail before launch. (Second from right) Four 1.5 U CubeSats will fit into a dispenser mounted on a rocket. Once in orbit, the CubeSats are released from the dispenser, activating a battery and triggering a 30-minute timer so that the satellites can get clear of the rocket and its other cargo before deploying. (Right) Full deployment involves raising a radio antenna (central helical structure) and unfurling four solar panels to power the satellite.

Perseus takes flight

A rapid-response satellite capability that is quick to build, easy to operate, and orders of magnitude lower in cost than traditional systems would enable many different types of missions and customers. For example, real-time data exfiltration from remote locations is an important mission, but has simply never been worth the astronomical costs, so to speak, of a dedicated satellite system.

In the spring of 2008, Andy Erickson, then in the Laboratory's Intelligence Community Program Office, began wondering if CubeSats might be the answer to a particular rapid-response nut he and his colleagues were trying to crack. Yes, CubeSats were thought of as basically toys, but that didn't mean their only uses were simple or trivial. Maybe with a little guidance CubeSats could step up and meet the challenge of modern national security needs. Spearheading the project, Erickson recruited Los Alamos colleague Steve Judd as project leader, and they spent the summer in a hot flurry of funding proposals, customer pitches, and preliminary research. By the fall they had secured initial funding, and the Los Alamos CubeSat effort, dubbed Perseus, was underway.

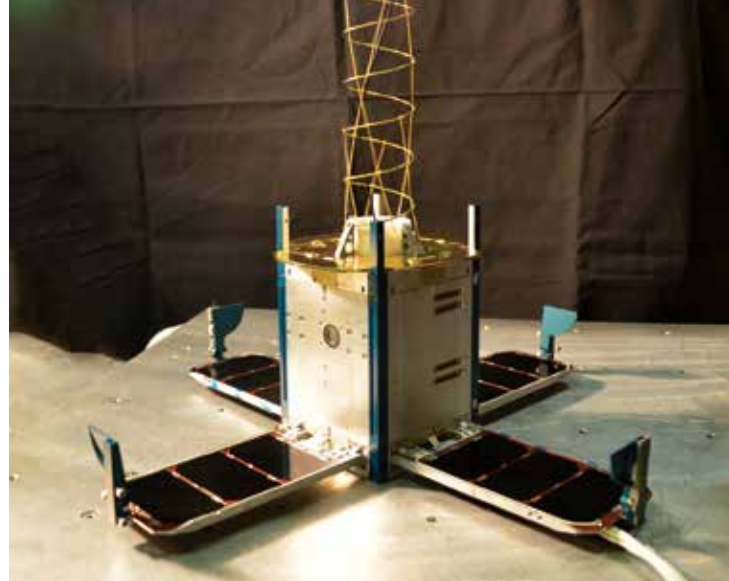
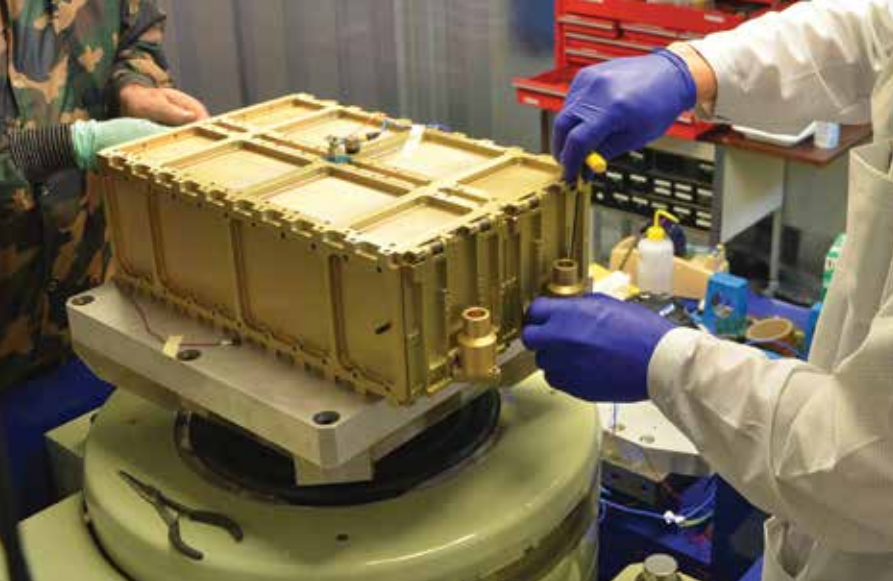
Having been handed a particular mission, Judd and the Perseus team quickly decided that miniaturizing a large satellite was the wrong tack and they needed an alternative, nontraditional approach. A breakthrough came when they realized that by building the entire system in-house at Los Alamos, from solar panels to circuit boards to software, using commercial off-the-shelf parts, they could drastically slash the time and money involved. In-house manufacture is rare in the satellite world; typically each component comes from a different specialty lab or collaborator, which can take cost and complications sky-high. The satellite that Erickson, Judd, and their small team built took just six months and had a jaw-dropping reproduction price tag of under \$20,000—that's more than a thousand times less expensive than the lowest-budget traditional satellite.

Their motto became "design to the mission, design as a system, and keep it simple." In other words, include only what's necessary to do the task at hand and design all components simultaneously. The basic machine they designed consisted of one circuit board, containing a radio, flash storage, and a microprocessor. With a quick software change it could be

On December 8, 2010, the SpaceX Falcon 9 rocket carried four Los Alamos project Perseus CubeSats into orbit 300 kilometers above Earth's surface.

CREDIT: NASA/Alan Ault





configured as a satellite, a ground station, or a field unit. When connected to a custom solar panel charger and a small monopole antenna, the satellite and the system were complete in a single stroke.

A radical departure from the norm, the Perseus system, consisting of satellites, ground stations, and field units, was so simple and seamless that non-expert users could operate it with just a few minutes of training. The ability to communicate from far away places in near-real-time was the main driver for the

On November 19, 2013, the Orbital Sciences Minotaur 1 rocket took eight second-generation Los Alamos CubeSats from Perseus's successor, project Prometheus, into orbit 500 kilometers above Earth's surface. Some Prometheus CubeSats are still on orbit, still online, and still on duty.

CREDIT: NASA/Chris Perry

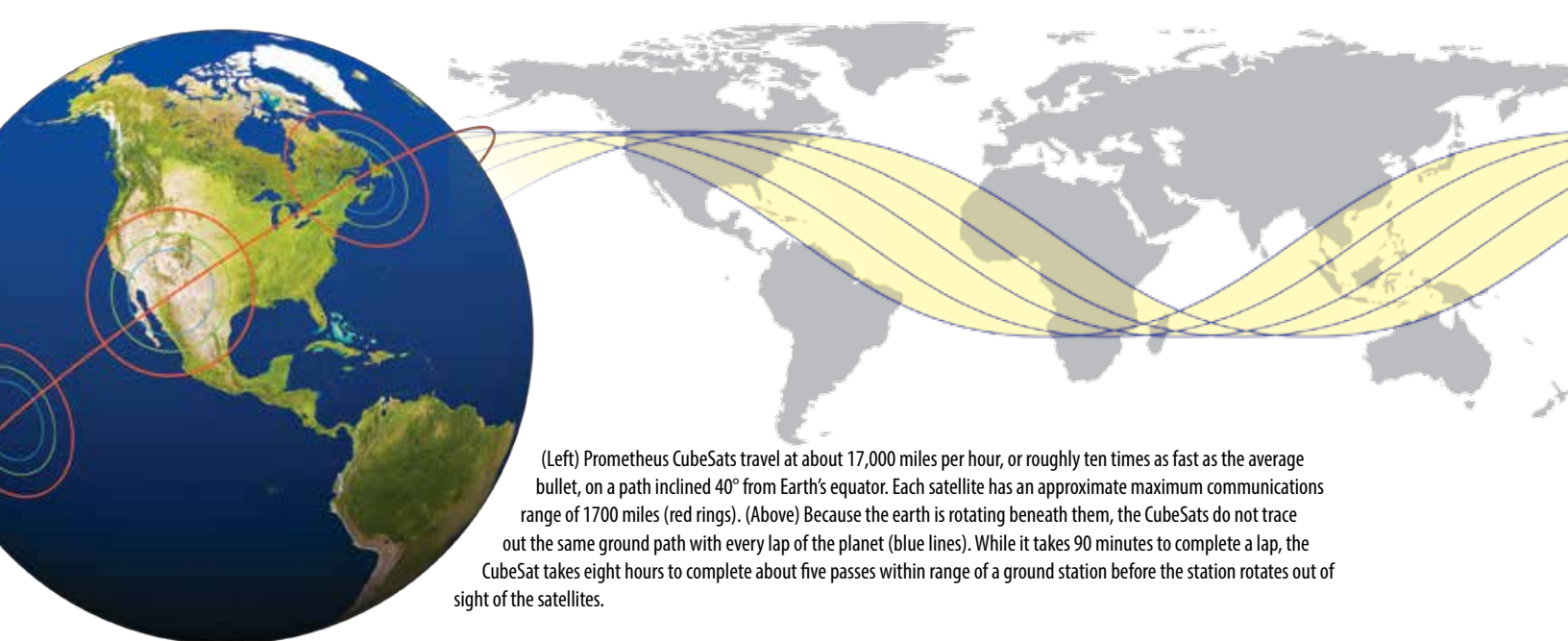


ground station design criteria of being low-cost, transportable and easy to set up. In the end, it too was shocking in both price (less than \$5000) and in profile. Small enough to be transported anywhere in the world by car or plane, a ground station could be set up and operational in about an hour. And since it contained the same custom-designed hardware and software that went into the CubeSat, the two were literally made for one another.

The first Los Alamos CubeSat went aloft in 2009 on a weather-balloon-type device to an altitude of 100,000 feet (more than twice the cruising altitude of a large commercial airliner). The balloon was launched in one location while teams in separate cars carried ground stations north, south, east, and west, to test communication capabilities from various distances as far as the next state over. After working out the bugs identified during the balloon test, four small Perseus flight units were chauffeured by sport utility vehicle to California for their reserved ride on a SpaceX Falcon 9 rocket, which launched in December 2010. Perseus was in flight.

It's not a matter of miniaturizing a big satellite, it's a matter of building the simplest satellite for a particular job.

"A lot of people said it wouldn't work," remembers Judd. The temperature extremes, energy demands, and size restrictions associated with traditional space components bred skepticism about how well these little satellites would actually work in space. But they did work. All four satellites deployed properly, linked to the ground station successfully on day one, and talked to the Perseus team daily for three weeks before leaving orbit and being destroyed—as planned—upon re-entry. (The "vacuum of space" mentioned at the beginning of this article, though illustrative, isn't technically accurate. The Perseus CubeSats were in an orbit about 300 kilometers



(Left) Prometheus CubeSats travel at about 17,000 miles per hour, or roughly ten times as fast as the average bullet, on a path inclined 40° from Earth's equator. Each satellite has an approximate maximum communications range of 1700 miles (red rings). (Above) Because the earth is rotating beneath them, the CubeSats do not trace out the same ground path with every lap of the planet (blue lines). While it takes 90 minutes to complete a lap, the CubeSat takes eight hours to complete about five passes within range of a ground station before the station rotates out of sight of the satellites.

above Earth's surface, which is on the outer fringe of its upper atmosphere. The drag created by atmospheric particles is what causes the CubeSats to leave orbit and fall toward Earth, gradually at first and then effectively all at once.)

The team, having been cautiously optimistic, was elated by the success. "It's still a satellite," says Judd, recounting his relief, "all the things that can go wrong with a big satellite can go wrong with a little satellite. Simple is not necessarily easy." Of course there were small glitches, but there were no fatal flaws. After proving successful at two-way and three-way communication, as well as the collection and relay of telemetry data, the proof of principle that CubeSats could provide a useful, cost-effective strategy for rapid response was official, and it was time to take it to the next level.

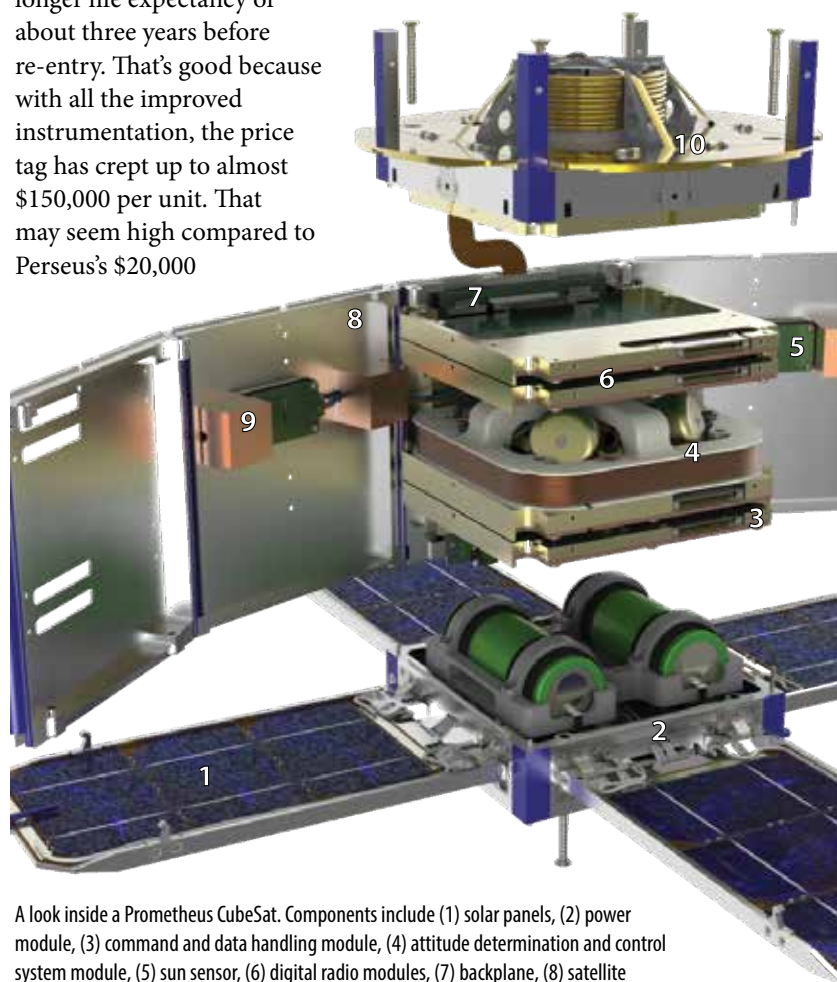
Prometheus unboxed

The second-generation Los Alamos CubeSat project, called Prometheus and led by Nicholas Dallmann, is considerably more sophisticated than its predecessor. The team too has expanded, now including more than 70 dedicated scientists from 13 Laboratory divisions. The Prometheus CubeSats are built on the basic Perseus architecture and are the same size as the Perseus CubeSats, 10×10×17 centimeters, or 1.5 U. (CubeSats typically range from the original 10-centimeter cube at 1.0 U up to 3.0 U.) But Prometheus units carry an increased power budget, higher-performance radio, bigger antenna, and more processing power, plus an attitude control system, magnetometer, gyroscope, and sun sensor.

For a project like this, the devil truly is in the details; every single component has to be meticulously designed. For example, there is a tiny motor for the CubeSat's attitude control (which direction it's pointing) that involves a tiny wheel. The axle hole must be precisely (but *precisely*) centered, otherwise the whole thing wigs out like an unbalanced washing machine. And the grease—they had to find a grease to lubricate the tiny wheel that wouldn't freeze but wouldn't evaporate in a vacuum either. All it takes is one element to fail for the whole device to fail—it can't be retrieved and fixed once it's been launched.

(Though CubeSats are far more disposable than traditional satellites, there are still considerable resources at stake and it's important to get it right.)

In November of 2013, eight Prometheus CubeSats went up on an Orbital Sciences Minotaur 1 rocket, and once again, all deployed and established contact on day one. They went to a significantly higher orbit than Perseus, about 500 kilometers from the earth's surface, which gives them a considerably longer life expectancy of about three years before re-entry. That's good because with all the improved instrumentation, the price tag has crept up to almost \$150,000 per unit. That may seem high compared to Perseus's \$20,000



A look inside a Prometheus CubeSat. Components include (1) solar panels, (2) power module, (3) command and data handling module, (4) attitude determination and control system module, (5) sun sensor, (6) digital radio modules, (7) backplane, (8) satellite structure, (9) ballast masses, and (10) cell phone-style camera not visible in diagram but located near the base of the antenna.

price tag, but for a sophisticated spacecraft it's still peanuts, and Dallmann is confident they can bring it down even more in the near future. With low overhead and 12 successful satellites over three years, compared to the historical average of about one small traditional satellite every five years, the CubeSats are definitely proving their worth.

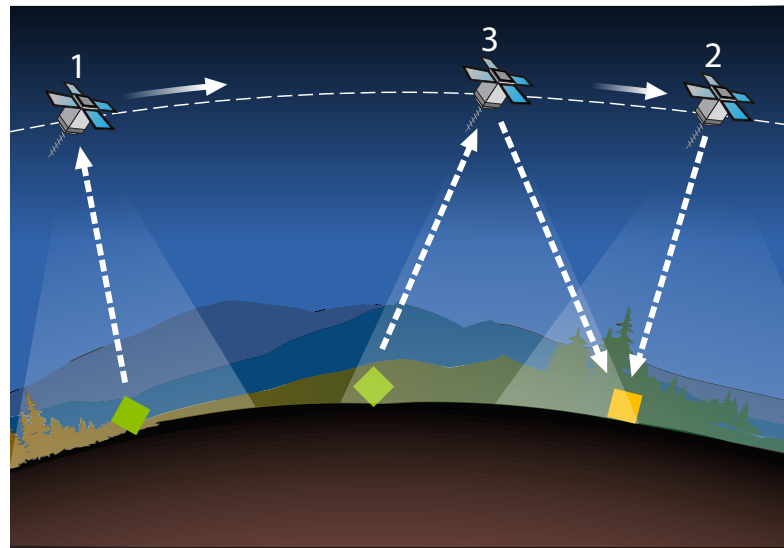
The Prometheus system is clearly a product of the technological times. Numerous aspects of it have only recently been made possible: some parts are custom-made by 3D printing; the system interface is on a web page; the ground station basically runs itself, sending a text message to its operator's cell phone if there is a problem; software updates transmit automatically when the CubeSat passes within range of its ground station, so there's no chance of missing the window; and the use of "cognitive radio," which automatically adjusts its parameters according to its environment, allows for very secure transmission encryption. There is more computing power among the eight tiny Prometheus flight units than on most active satellites as a result of the very modern parts used to make them. The evolution of off-the-shelf components, most of which are getting stronger, smaller, cheaper, and more easily integrated every year, has enabled a true satellite revolution.

CubeSat constellation

The Prometheus team refers to its array of CubeSats as a constellation of satellites. From this definition, their strength and novelty is evident: together they form a set of unique, specialized, highly compatible, and synergistic tools. They encircle the planet in single file, with each satellite completing a lap around Earth every 90 minutes. Although they travel within a fixed plane, the earth is rotating underneath the plane, so the satellites don't trace out the same ground path with every lap. When a CubeSat's path takes it within range of a ground station it's called a pass. The best passes are when the CubeSat travels almost directly over the ground station, thereby minimizing the distance between the two. A poor pass is one in which the CubeSat passes just above the horizon at maximum still-visible distance from the ground station—any further and it would be out of range. Every time a CubeSat comes around to a given ground station, the first pass (approaching) is usually poor, followed some time later by a mediocre pass, then the best pass (closest to directly overhead), then another mediocre pass on the other side, and finally another poor pass as the CubeSat's orbit travels out of range of the ground station. It takes roughly eight hours, with a 10–15 minute pass every 90 minutes, for a CubeSat to travel first into and then out of range of a ground station or field unit.

Over-the-horizon communication is one of the main functions of the Prometheus system. There are two ways in which it fills the bill. The first is called store-and-forward. In this mode, a sensor in the field (e.g. a camera) sends information to a CubeSat as it passes within range.

The CubeSat then holds on to the information until the receiving ground station comes into range, at which point the ground station downloads the information from the CubeSat. This mode is unconstrained by



There are two modes of over-the-horizon data exfiltration that Prometheus performs. In the store-and-forward mode, the CubeSat collects data (1) from a remote field sensor (green diamond), then transmits the data (2) to a distant ground station (orange square) at some later time. In the near-real-time mode, the field sensor and ground station are not within range of each other but are within range of the same CubeSat (3), which can bounce the data almost instantaneously from the sensor to the station.

distance—the CubeSat can hold the data for as long as it takes to arrive at the right ground station—but it isn't the most expedient because the data can only travel as fast as the CubeSat itself.

A faster mode is called near-real-time and basically uses the CubeSat to bounce information over the horizon. For near-real-time communication, the field sensor and ground station have to be in approximately the same region—a sensor in Norway and a ground station in Nebraska won't work, but a sensor in Los Angeles and ground station in Los Alamos will work well. When the field sensor and ground station are regionally close but still out of range of one another (over the horizon), a CubeSat passing within range of both can relay information almost instantaneously. This method is faster than store-and-forward, but it's constrained by distance. However, with considerable effort and creativity, the team got their CubeSat's range up to 1700 miles, or almost half the distance across the continental United States. And since the ground stations are low in cost and high in user friendliness, they can be popped up as needed just about anywhere. So the distance constraint too was made manageable by the mission-driven CubeSat team.

Above and beyond

Although the Prometheus CubeSats are still going, Dallmann and the Prometheus team are already hard at work on the third generation of Los Alamos CubeSats, which they refer to as Prometheus block 2. With the block 2 CubeSats will come even more refinement and efficiency. Many things will be similar, but practically nothing will be identical—it will all be better. The solar panels will be twice the size (but cleverly

won't increase the volume of the stowed CubeSat), attitude control will be improved, and additional sensors will be added. The ground stations, too, will be similarly upgraded. "There are marvelous electronics now," muses Judd, now a consultant on the project. "With the reliability of modern techniques they can really crank them out, making 20, 30, or even 40 in a year." The team could make 40 CubeSats this year alone, but they probably won't need to; block 2 is projected to consist of 10 CubeSats slated for launch sometime in the summer of 2016.

The ability to mass-produce its CubeSats was a key goal for the Prometheus team from the get-go. And an important step toward that goal, now underway, is the transfer of its unique CubeSat technology to industry. The team's minimalist, in-house approach has opened up a whole new set of potential missions and customers, with all of the U.S. armed services and numerous private companies now investing in CubeSat research. One way that block 2 CubeSats will be competitive in the private sector is the plug-and-play aspect of their new hosted payload option. The payload is a special compartment that can be connected to the CubeSat and customized to a particular mission through modification of the contents. What type of technology or sensor goes in the payload will be decided by the customer, who can then focus on its desired data product and skip worrying about the nuts and bolts of the satellite itself.

Prometheus technical lead Nick Dallmann inspects a ground station near Los Alamos. The ground station is designed to be set up in the field and operated by a single nonexpert user in under an hour.



As if all of their empirical successes weren't accolades enough, the Prometheus team was chosen this year to receive the U.S. Department of Energy Secretary's Honor Award. This is the highest internal non-monetary recognition that Department of Energy employees can receive for their service and contributions to the mission of the Department and to the benefit of the nation.

CubeSats are reliable, practical, malleable little tools.

The Prometheus effort is part of a larger program at Los Alamos, the Agile Space Program, which is concerned with new, low cost, rapidly deployed space systems. While CubeSats are the smallest satellites in this program, they aren't the only ones. Most of the systems that have been perfected for Prometheus can be easily scaled up to larger (but still small) satellites. Having already invested the time and effort to develop CubeSat technology, the Agile Space Program stands to reap tremendous reward from other small satellite applications.

When CubeSats first came on the satellite scene, nobody knew that they could bring about a revolution in space-based communication (and, by extension, to the intelligence, surveillance, and reconnaissance tools that rely on that communication). But with some out-of-the box (inside the box?) thinking, they have stepped up as reliable, practical, malleable little tools ideal for nontraditional jobs. And since their lifespans are limited, they will always be new, always be modern, and never become dark hunks of space junk, drifting through eternity. CubeSats, it seems, have proven their mettle and earned some respect. So too has everyone on the Prometheus team. As Dallmann emphasizes, "We are a team; there is no member who is more important or deserves more credit than the others." So, in a way, the team itself is like a fleet of CubeSats. With each member doing a specific task, quickly and competently, the team comprises a machine that is much, much greater than the sum of its parts. **LDRD**

—Eleanor Hutterer

More satellite research at Los Alamos

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www.lanl.gov/discover/publications/1663/issues-archive/june2012.pdf
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WHAT'S LACKING WITH FRACKING

THE FUEL-extraction method behind the U.S. energy boom gets new science to mitigate wastewater and other environmental concerns while improving efficiency.



U.S. CARBON EMISSIONS ARE DECLINING. In the past ten years, per-capita emissions of carbon dioxide have dropped to a level not seen since the 1960s, attributed in large part to a recent surge in natural-gas production. With natural gas becoming cheap and abundant, electrical power generation has partially shifted away from coal. And because natural gas generates only about half as much carbon dioxide as coal for every watt of energy produced, the nation is putting less carbon into the atmosphere—all while stimulating the economy and raising the possibility of U.S. energy independence.

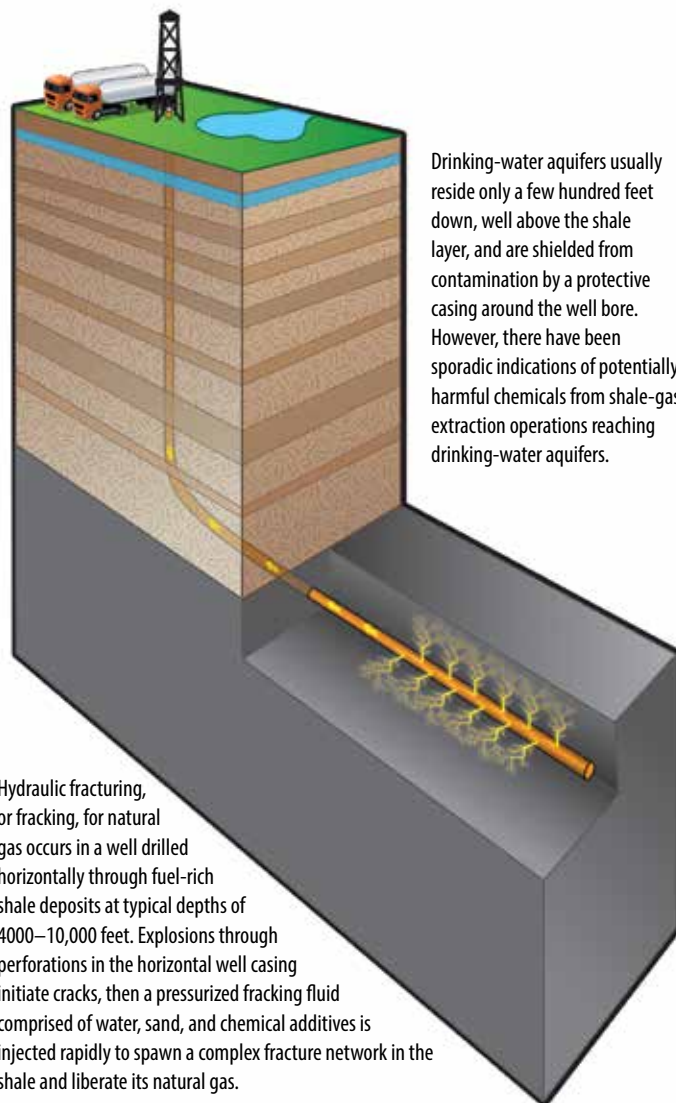
The trouble is, most of this natural gas has been coming from shale formations more than a mile underground, and there are distinct technical and environmental challenges associated with getting it out. Currently, such operations extract only about 15 percent of the natural gas in place and annually consume about a hundred billion gallons of freshwater to do so, turning much of it into highly toxic wastewater too expensive to remediate. The wastewater is usually re-injected deep underground, just to get rid of it. But both the fuel extraction and wastewater reinjection create the risk that toxic fluids could migrate along defective wellbores, or natural faults and fractures, into drinking-water aquifers. In addition, wastewater reinjection has been shown to cause low-level earthquakes. By increasing the pressure in subsurface pores, the process can increase seismicity in regions with stressed, preexisting faults.

Not surprisingly then, the most successful method of shale-gas extraction, known as hydraulic fracturing, or fracking, is fraught with controversy. Even the most cursory of internet searches on the term instantly reveals a flurry of opposition—and opposition to the opposition. The controversy, however, is somewhat misplaced.

Fracking operations typically leave 80–90% of the available fuel in the ground.

“Fracking itself is not the problem,” says Los Alamos earth and environmental scientist Hari Viswanathan. “That deep underground, the fractures don’t extend far enough upward to penetrate drinking-water aquifers. It’s the large-scale industrial operations at the surface, the potential leakage paths formed by wells, and the disposal of wastewater that create the problems.”

Viswanathan leads a multidisciplinary team of expert scientists, postdoctoral researchers, and students in a broad effort to develop the interconnected science—the mechanics, chemistry, thermodynamics, and hydrodynamics on scales ranging from nanometers to kilometers—of how fracturing really affects the deep geological formations. His hope is that it will lead to better environmental security, in terms of subsurface oil and gas movement, and substantially more efficient extraction of shale gas. That would mean fewer wells producing more gas per well, which would lower the overall



Hydraulic fracturing, or fracking, for natural gas occurs in a well drilled horizontally through fuel-rich shale deposits at typical depths of 4000–10,000 feet. Explosions through perforations in the horizontal well casing initiate cracks, then a pressurized fracking fluid comprised of water, sand, and chemical additives is injected rapidly to spawn a complex fracture network in the shale and liberate its natural gas.

water use, lower the wastewater injection and associated earthquakes, and lower the risk of groundwater contamination—all while obtaining more of a relatively clean-burning fuel.

How fracking works

“Hydraulic fracturing for shale gas is a clever way to extract what has long been an inaccessible resource,” Viswanathan says. “You can’t just draw it up because the gas is trapped inside a low-permeability rock. Nothing flows from it.”

The solution in use today involves a number of innovations, beginning with a very deep well that drops straight down and then slowly arcs to run horizontally through the heart of the shale layer. Explosive charges along the horizontal section create perforations through the well casing and cut into the shale formation. Then a pressurized mixture of water, sand, and chemicals is injected in a rush to frack the rock, generating a rich network of fractures. If the process is successful, fuel will be able to move through the fractures.

Lowering the pressure at the well head generates suction that may lead to years of natural gas production, as long as the fractures remain open. However, these shale formations often reside 8000 feet below the surface, and the weight of all that overlying rock tends to squeeze the fractures closed again.

That's why sand is included in the fracking fluid. The sand is selected to have an ideal grain size for propping open the fractures once they have been created and, for that reason, is referred to as a proppant, or propping agent.

In addition to the proppant, chemical additives are included in the fracking fluid. Biocides prevent microbial activity, and soapy surfactants reduce the fluid's viscosity, allowing more energy to be delivered to the fracture tips for a better fracture network overall. Unfortunately, the use of these chemicals, some cancer causing, also introduces the danger that they might find their way into drinking-water aquifers. Indeed, an Environmental Protection Agency (EPA) report out earlier this year finds examples of drinking-water contamination due to fracking operations, stemming both from surface spills and fluid migration along defective wellbores. Yet the report shows that the contamination identified so far is quite limited and finds no "widespread, systemic impacts on drinking water resources in the United States."

As Viswanathan explains, chemical additives shouldn't be considered the only source of contamination risk anyway, regardless of their movement underground, because the toxin-infused fluid drawn back up from the well is generally worse than the chemicals that were sent down. Fracking water withdrawn during the well's productive life contains large quantities of naturally occurring salts, heavy metals, and radioactive elements from deep underground, in addition to the original additives. So the objective of protecting the environment, as Viswanathan sees it, shouldn't just be about reducing additives; it should be about reducing water use altogether.

Sweep and scour

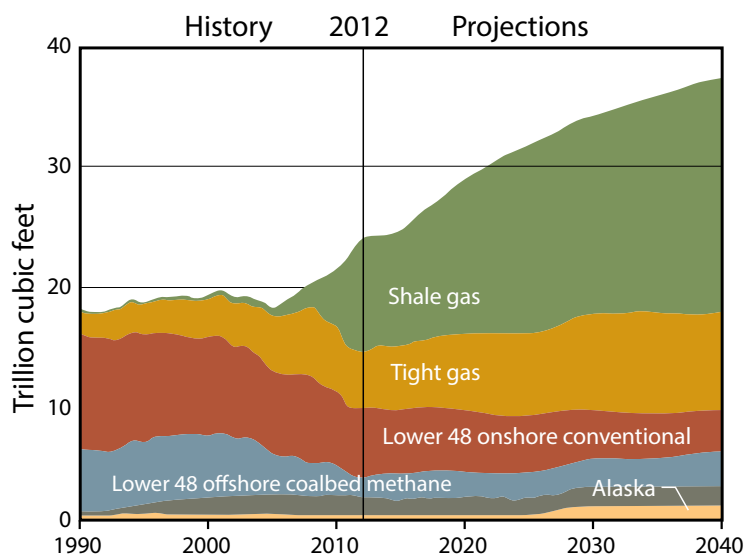
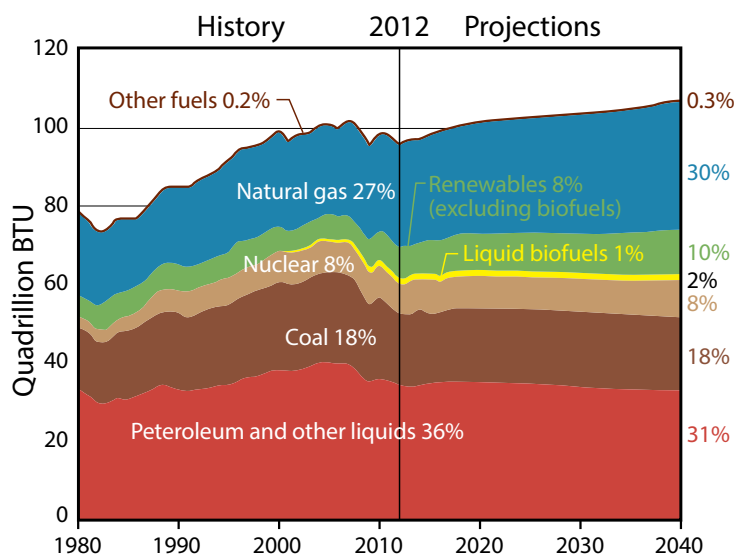
Deep-shale deposits are a compressed blend of fine-grained rock, natural gas, and hydrocarbon oil (also valuable). Neither the oil nor the gas generally resides within large open holes in the rock; rather, they occupy naturally existing

fractures and tiny pores. They also exist in a form chemically adsorbed to other organic molecules in the rock.

Ideally, fracking operations tap into all of these locations. First, fracking-induced fractures link to existing fractures and access the fuel from them; this is the low-hanging fruit of the fuel-from-shale world. Once the fuel is drawn from the in-place fractures accessed by the initial fracking, it might then be drawn from an extensive network of mechanically damaged rock surrounding the primary fracture network. Then hopefully the fracture-damage zone allows the fracking fluid to sweep through to access small pores and, when drawn back out, gather their fuels. Over longer periods of time, the fluid could desorb fuels attached to solid organic matter and pull those out as well.

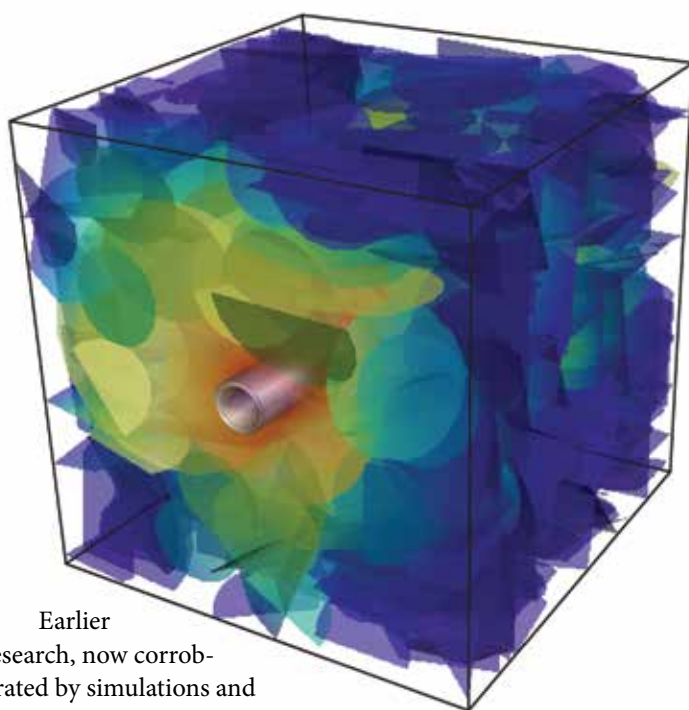
This idealized progression seems consistent with industry experience. Fuel production dwindles rapidly during the first few years, presumably as larger, existing fractures are drained, and smaller pockets feed the well more slowly. Nonetheless, in the end, fracking operations typically leave 80–90 percent of the available fuel in the ground. In some cases, oil and gas operators may be able to get more fuel out by refracking an existing well after a few years. But the gas recovery remains inefficient overall, and a significant reason for that turns out to be the fracking water itself.

When water is injected to frack a well, the desirable outcome of establishing fractures is accompanied by two undesirable outcomes, which may inhibit access to all but the most easily accessed fuel within the shale. First, the shale rapidly soaks up most of the water like a sponge, causing it to swell and therefore closing the fractures, both natural and man-made. Second, water fills in the fractures, effectively sealing off the fuel inside because of water's high surface tension and the fact that it doesn't mix with hydrocarbon fuels (like oil). Both inhibiting effects are more pronounced in the smaller fractures within the network and could be minimized by choosing another fluid instead of water.

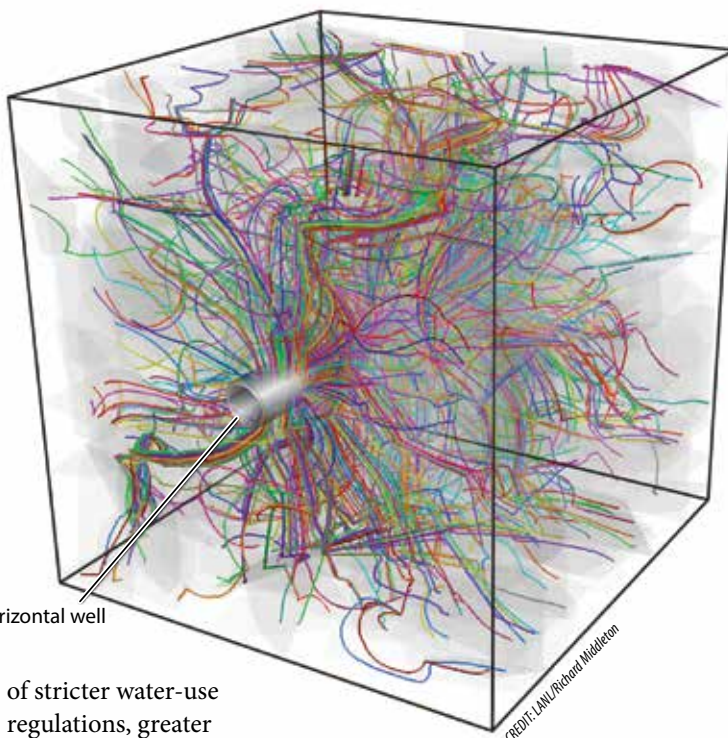


(Left) In 1990, natural gas made up 23 percent of American energy consumption, but that share has been rising, partially displacing coal and petroleum in recent years. By 2012, natural gas made up 27 percent of American energy consumption and is projected to reach 30 percent by 2040. (Right) Shale gas, mostly from fracking, was a negligible source of natural gas in 1990 but by 2012 exceeded all other individual sources and is projected to exceed all other sources combined by 2040.

CREDIT: Energy Information Administration



High-performance computing simulation of fracking-well operations: (Above-left) Slivers represent existing cracks in the shale that harbor natural gas and other hydrocarbon fuels. Fracking produces additional fractures, extending outward from the horizontal well. The man-made fractures intersect with existing cracks and create a path for fuel to flow into the well, and an applied pressure gradient (indicated by color) drives the flow. (Below-right) Hundreds of fuel-flow trajectories are identified, allowing researchers to compute the natural-gas production rate over time.



Horizontal well

CREDIT: LANL/Richard Middleton

Earlier research, now corroborated by simulations and experiments from Los Alamos, suggests that a fluid based on supercritical carbon dioxide (scCO_2), with attributes of both gas and liquid, could prove more effective in a variety of ways. Initially, it may be able to produce a more elaborate and extensive fracture network than water because when it expands into a new volume, it cools like gas expanding from a spray can, and thereby generates thermally induced fractures. That means an scCO_2 fracking fluid should generate more fractures than water as it moves through the shale. More research is needed to confirm this—and don't worry, Viswanathan is working on it—but even if water initiates the fracking and remains in place, scCO_2 can still be used in a secondary process, moving through the water to help extract the fuel.

Compared to water, scCO_2 also has less of a flow-blocking effect due to its lower surface tension and its miscibility with hydrocarbons. Natural gas in pockets trapped by water would instead dissolve into scCO_2 . And scCO_2 even displaces chemical bonds that cause natural gas molecules to adhere to organic matter in the shale. Effectively, it sweeps the fuel from inside the fracture network and scours it from the walls. Perhaps more important still, its use could greatly reduce (or even eliminate) the need for risky chemical additives and greatly reduce (or even eliminate) the production of toxic wastewater that is currently re-injected underground. And if the scCO_2 must be re-injected, that solves another problem by keeping it out of the atmosphere.

On its own or mixed with water, scCO_2 has been used in oil and gas drilling in the past and is sometimes used today to extract more gas than water alone. Results have been inconsistent at times, but in previous experiments sponsored by the Department of Energy (DOE), the use of scCO_2 has increased natural gas production by up to five times over water alone while dramatically cutting water consumption.

So why is water still the fluid of choice? The simple answer is price. Right now, water, even drinking-quality water, is much less expensive than scCO_2 in the quantities needed for fracking operations. However, that may change in the face

of stricter water-use regulations, greater application of carbon capture and storage technology, or both. Indeed, these issues are central themes of two DOE crosscutting initiatives, SubTER (subsurface technology development for energy security and environmental responsibility) and the Water-Energy Nexus (interdependence between water and energy resources). But even under existing water and carbon regulations, the price-motivated choice of water for fracking could change in the face of a new scientific prediction capability that allows natural gas companies to recover the lion's share of the fuel left in place by their current operations.

"I think we are on our way toward demonstrating an economics of natural gas production that actually favors smaller environmental impacts," says Viswanathan. "We just need realistic calculations—and experiments carried out under realistic conditions to validate them—to show us the way there."

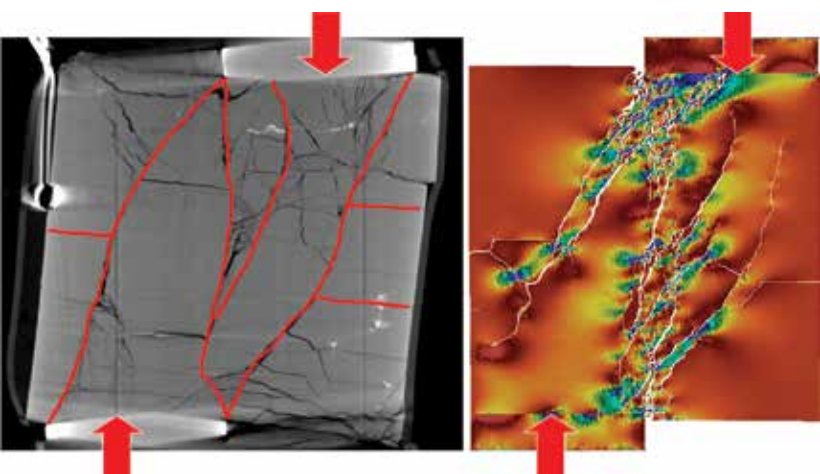
Crack team

Satish Karra, Esteban Rougier, Mark Porter, and Robert Currier are fluid flow, rock mechanics, and chemistry researchers on Viswanathan's team. They are responsible for crafting a detailed computer simulation of fractured natural-gas systems deep underground and generating critical experimental data to feed into it. The idea is, if the simulation accounts for all the relevant processes, then it can answer all the what-if questions one might ask to work out the best way to obtain the most natural gas with the least environmental

risk. What if we apply X amount of pressure and cycle it up and down? What if we use a 60–40 mixture of water and scCO_2 ? What if we change proppants and maybe re-frack periodically?

The simulation is complex because it must take into account a variety of physical processes occurring across an enormous range of size scales. Karra, for example, has focused heavily on the scale of the overall shale reservoir, analyzed over the kilometers surrounding the well site. Rougier, by contrast, studies the core scale, ranging from a hundred-thousandth of a meter up to several meters and representing fracking features in the immediate vicinity of the well. Porter examines other scales that extend much smaller, to millionths and even billionths of a meter, representing micro-fractures and tiny natural pores in the shale, respectively. Each scale corresponds to a different set of key processes—e.g., fracture propagation at the core scale and multiphase fluid dynamics at the micro-scale—and all of this must feed into the simulation for accurate results.

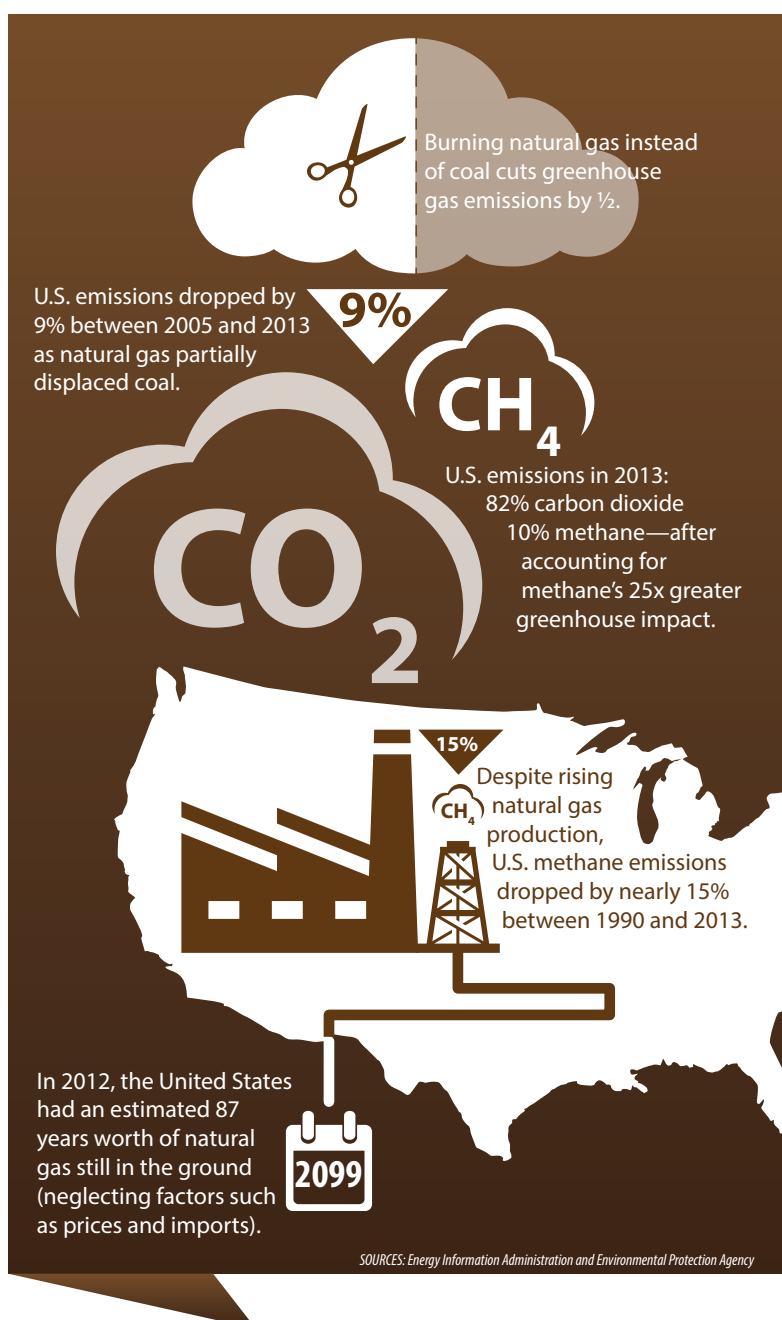
Karra begins with a model of the reservoir geology surrounding a horizontally drilled well. He programs his simulation to include a number of simplified, preexisting planar fractures at various angles within the shale. He then simulates the effect of fracking by establishing new fractures that extend radially outward at regularly spaced intervals along the well. These man-made fractures intersect the preexisting, natural ones and thereby access the natural gas trapped within them. To simulate drawing the gas out, he creates a pressure gradient and, by taking into account pressure, aperture, and porosity effects, calculates flow rates and predicts natural-gas production over the operational life of the well. But unlike existing computer models already in use by industry, which tend to rely on overly idealized conceptions of the reservoir or simply impose the observed outcomes from other well sites, Karra's simulation is built upon first-principle, computational physics grounded by reliable fracture datasets to guide the core-scale activity.

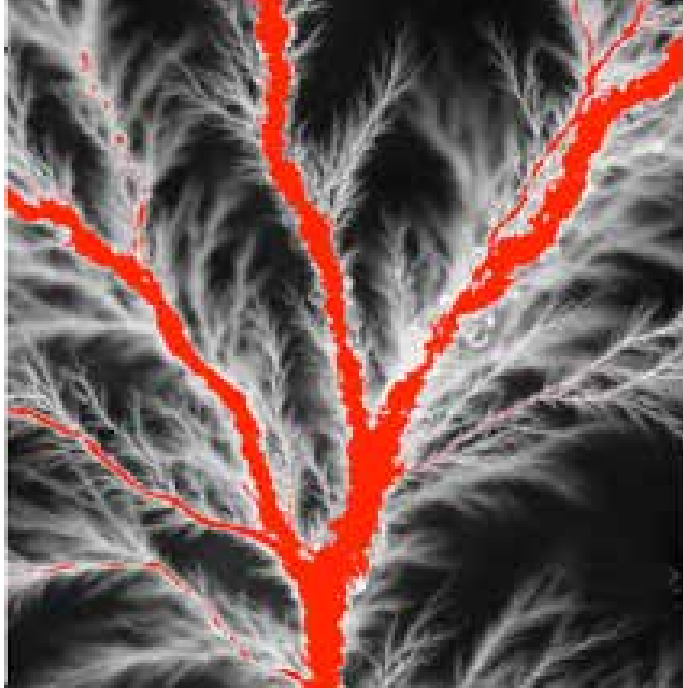


X-ray computed tomography image (left) and computer simulation (right) of fracturing produced by applying a shear force (red arrows) to an industry core sample of drilled shale. The experiment is carried out in a containment vessel at high temperature and pressure conditions, representative of those occurring in deep-shale deposits. Since the pressure exerts a force from all sides, in all three dimensions, researchers call this a triaxial experiment. X-ray imagery like this is used to improve the accuracy of the simulation to better predict shale fracturing under different conditions.

These reliable fracture datasets have to come from somewhere, and that's where Bill Carey, a Los Alamos oil-and-gas expert, comes in. Carey begins with a cylindrical core sample of shale, 1–3 inches long and 1 inch in diameter, provided by industry partner Chesapeake Energy. Then he subjects it to three-dimensional stresses in what's called a triaxial experiment to induce realistic hydraulic and shear fracturing within the sample. He has pioneered a unique capability to accomplish this within a high-temperature, high-pressure containment vessel housed inside an x-ray computed tomography system to observe fracturing directly at the actual conditions found in deep-shale reservoirs, including how the shale soaks up water.

Rougier uses these fracture-experiment results to calibrate a core-scale, finite-element computer simulation of the process. When the simulation correctly produces a nearly identical fracture network from the same stresses imposed on the





Oil (shown in red) being pushed into a laboratory-synthesized fracture network floods large channels but does not reach into dead-end extremities, implying that relevant fluid behaviors like capillary action and surface tension cannot be ignored when predicting flow in and out of the large number of small fractures.

physical sample, Rougier knows he's got the fracture physics right. Then his simulation can be used to predict fracture propagation under different fluid compositions, rock characteristics, and injection schemes.

In addition, Carey measures the permeability of the sample—still in the pressurized experimental apparatus—from which he and Rougier can calculate fuel extraction rates. As expected, the measured permeability is zero until fractures form, then spikes up and diminishes with time as the unrelenting pressure squeezes the fissures closed. These permeability results, too, are incorporated into the core-scale computer simulation, and the core-scale simulation is incorporated into the reservoir-scale simulation. All together, the simulation correctly reproduces the production curve—depicting natural-gas extraction over time—obtained from industry experience. The curve climbs rapidly upon initial fracturing and drops away as the permeability declines over the following years. However, the simulated curve shows less production than what actually occurs in the later years.

“Our simulation doesn't yet include the micro- and nano-scale effects that govern natural-gas production after the larger pockets have been emptied,” explains Viswanathan. “We need data to characterize that as well.”

The little things

Porter, Currier, and Carey are addressing that objective with a series of microfluidics experiments, which are just what they sound like: fluid-flow tests using tiny channels, representing the channels where much of the shale gas is trapped. The data they obtain will be merged into the overall simulation to better explain production in later years and provide a more complete basis for assessing the likely impacts of various proposed improvements to the process.

In a simple initial experiment, Porter and Currier created an idealized fishbone-patterned fracture network in a microfluidic wafer made of shale. They saturated it with oil and then drove water through it with a pressure gradient along its spine. The water did not penetrate into the side channels and therefore demonstrated its inability to sweep out hydrocarbon fuels from dead-end fractures. The team also made an advanced fluid-dynamical computer model of the same setup and verified its ability to match the results of the experiment, including the detailed shape of the water “finger” making its way through the oil.

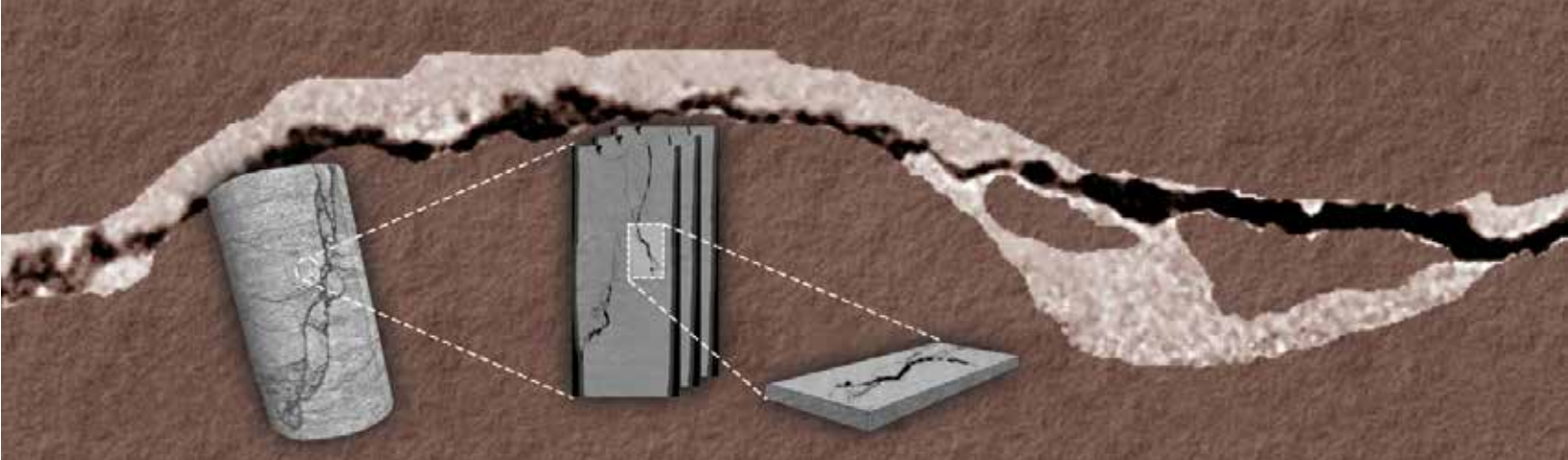
But realistic fractures are better than idealized ones, so Porter, Currier, and Carey perform sophisticated x-ray and neutron tomography on the fractured samples from the triaxial experiments and, using the resulting imagery as a guide, etch their actual fracture patterns into microfluidic shale wafers. Then they push different fluids through, including oil, water, and scCO_2 .

When they tried pushing oil through a complex fracture network, the oil didn't reach the network's narrow, dead-end extremities due to micro-scale fluid-physics effects: surface tension, capillary forces, wetting properties of the rocks, and the like. These are evidently very important at small scales. And when they tried injecting water followed by scCO_2 into a real fracture network etched in shale, they observed the scCO_2 tunneling through the water in a distinctive fashion, demonstrating that the different fluids have very different capabilities within fractured shale. Discoveries from microfluidics experiments like these, together with other results on even smaller scales, will be added to the overall multiscale permeability calculation within the reservoir-scale fracking simulation.

**We may discover an economics of
natural-gas production that actually
favors smaller environmental impacts.**

“The science of hydraulic fracturing for hydrocarbon fuel is surprisingly difficult to uncover,” says Viswanathan. “It's tremendously important, for example, that we've learned how to carry out our experiments, both fracturing and microfluidics, under actual reservoir temperatures and pressures. The fluid and wetting properties that dominate the fuel-sweep interactions depend greatly upon those temperatures and pressures. And as for scCO_2 ,”—he spells out the letters rather than voicing ‘supercritical carbon dioxide’—“well, CO_2 wouldn't even be sc without the high T and P”

It was no easy task to conduct realistic experiments at actual reservoir conditions; it took nearly five years to develop the necessary techniques, combining a variety of disparate Los Alamos capabilities from well beyond Viswanathan's Earth Sciences office suite—capabilities like high-performance computing, neutron tomography at the Los Alamos Neutron



Fractures produced in real shale during triaxial experiments (see image on page 29) and revealed by microtomography are etched into shale wafers for microfluidics experimentation. Here, water (gray-tan) fills a fracture, and subsequently injected supercritical carbon dioxide (black) displaces its way through the water to access potential natural-gas pockets. Alternate fluids like supercritical carbon dioxide may prove more efficient and more environmentally friendly than water if they can be made cost effective.

Science Center, and microscopic etching at the Lab's Center for Integrated Nanotechnologies. But now, after a decade of groundwork (so to speak), he is ready to get some answers: how water hinders fuel extraction, whether alternative fluids can deliver better performance or reduced swelling, and what the overall permeability of fractured shale is. His team is at the forefront of all these things.

Subsurface crossroads

The shale-gas industry has been slowly improving its extraction efficiencies—getting more gas out—by brute force, drilling longer horizontal wells and placing more fracture-initiation stages along their length. But Viswanathan says there is a sentiment in the field that these sorts of improvements have already maxed out. It is only through a genuine quantitative science of fracking that further improvements of any real significance are likely to materialize.

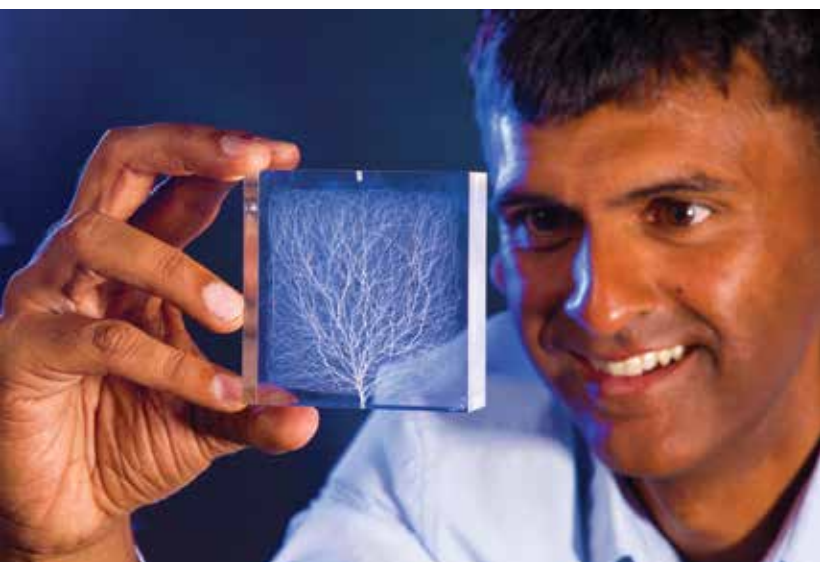
That same new science also appears to be the nation's best near-term hope for mitigating environmental dangers while reducing carbon emissions from burning coal. A substantial

reduction in fracking water use (and therefore wastewater production) is unlikely until better knowledge is available to inform alternate-fluid practices and higher-efficiency extraction strategies. And more reliable containment of fracking-well toxins, protection of drinking-water aquifers, and even safeguards against atmospheric leaks are unlikely without a more developed science of fracture generation and propagation. (Pound for pound over a 100-year period, natural gas is 25 times more potent than carbon dioxide as a greenhouse gas, according to the EPA. It would be a shame to ruin the lower carbon-emission rates achieved in recent years because of gas leaks reaching the surface.)

Unknowns remain, of course. Small-scale effects have yet to be fully accounted for in Viswanathan's simulations, and different fracturing methods—using still other fracking fluids, such as nitrogen, or none at all and explosives instead—have yet to be sufficiently studied. In addition, his new subsurface science has yet to be repackaged in earnest for other energy contexts beyond fossil-fuel extraction, such as carbon capture and storage, geothermal energy, and underground nuclear-waste repositories. But the potential to advance each of these energy applications is definitely there, as is the remarkable potential for national energy independence.

With so much riding on a science-based predictive capability for deep drilling, there's no question: when it comes to establishing the science and putting it to use, it's time to get cracking. **LDRD**

—Craig Tyler



Hari Viswanathan inspects a microfluidic cell used to study the extraction of hydrocarbon fuels from a complex (and in this case, synthetic) fracture network.

More subsurface energy and environmental research at Los Alamos

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spotlights

Positive Vibes

Now hear this: Sound waves allow researchers to see deep inside objects too difficult or dangerous to cut into for a direct look. The Laboratory's Dipen Sinha has made a career of it, pioneering one successful application after another, and is now working toward his crowning achievement to date, using sound waves to treat—not just diagnose, but treat—just about every manner of debilitating brain condition commonly known.

What began during the first Gulf War with acoustic techniques to scan for chemical weapons inside unexploded munitions has since evolved into a series of imaginative solutions to other vexing peer-inside problems. Sinha developed acoustic methods for assessing how much water, oil, or natural gas is produced from any oil well. He subsequently aimed sound beams at eggs to identify those carrying salmonella. He worked out a way to test for glaucoma by measuring vibrations caused by collimated sound waves impinging imperceptibly on the eye. He upgraded biological laboratory research by adding acoustic capabilities to flow cytometers—machines that separate cells of different types from a mixed tissue sample. Then he turned his attention to the human brain.

Initially, Sinha showed that he could measure intracranial pressure (ICP)—the fluid pressure in the brain—using sound transducers placed against the subject's temples to produce and measure microscopic, ICP-dependent vibrations from the skull. Elevated ICP is often the key piece of information needed to properly diagnose life-threatening, combat-related and other head-trauma injuries, but the current method of monitoring it requires an enormously risky procedure. Doctors must drill into the skull and insert a catheter deep into the brain's interior, exposing the patient to a serious risk of potentially fatal infection. Yet Sinha's acoustic vibrations, imperceptible to the patient, provide ICP monitoring with none of the risk. They even reveal subtle changes in the ICP caused by, for example, a simple tilting of the head—such as when a driver begins to nod off at the wheel.

But sound waves are good for more than just noninvasive measurements in the brain. They can actually stimulate neurons with acoustically driven pressure waves, causing them to fire in much the same way as electrode-delivered impulses do. And that opens the door to a whole slew of potential medical advances.

"We in the field can already trigger neurons in a petri dish with sound," says Sinha. "And we already have good evidence that equivalent electrical stimulation can relieve a number of serious disorders—including Parkinson's disease, chronic pain, and deep depression—and even increase creativity. It's not such a big leap to expect the same treatment to work with sound beams, without all the complications associated with inserting electrodes into the brain."

Sinha refers to a neurosurgical technique known as deep-brain stimulation (DBS), which is just what it sounds like. In practice, electrodes placed deep in the brain are connected to wires leading to the cranial equivalent of a pacemaker. The device generates controllable electrical signals designed either to disrupt overactive brain circuits or

stimulate underactive ones, wherever they may reside. For the tremors of Parkinson's disease, the electrodes are placed in the thalamus; for depression, in the mood center of the brain known as Area 25; for Alzheimer's disease, in regions associated with memory, cognition, or neurotransmitter activity. (DBS treatment is currently approved for Parkinson's and other movement disorders as well as obsessive-compulsive disorder; it is currently under study for depression, Alzheimer's, and chronic pain.) Not surprisingly, the success of DBS relies on properly positioning electrodes within the problem area of the brain.

With sound waves, one or more acoustic generators would be set up against the head and aimed at the problem area inside the brain. This produces two significant difficulties, however. The first is getting the sound waves through the skull, although Sinha has already overcome that hurdle with a highly collimated ultrasound source that, unlike other sources, produces a beam whose shape does not depend on the sound-wave frequency. That allows him to project low-frequency waves capable of penetrating the skull along a narrow column across the brain.

Of course, that's not good enough; the sound must be restricted to a small target area in the brain and not an entire column through it. That's the second difficulty. But Sinha has that one covered too. With a technique called parametric mixing—Sinha has seven patents for this—two crossed beams deliver the desired acoustic signal to their intersection point only. In essence, this method of sound-wave targeting could allow different people to listen to different music in the same room, and in the brain, he believes it will produce reliably targeted stimulation (or disruption, as needed) for misfiring neurons. As an added bonus, he notes that the stimulation is highly adjustable in terms of sound modulation and energy delivery, allowing doctors to optimize the treatment settings for each patient.

Sinha is not yet experimenting with actual brains, so there is much research yet to be done. But if successful, his work could spawn a welcome shift in the treatment of serious mental disorders from expensive and dangerous surgeries to comparatively inexpensive and noninvasive sonic headgear.

—Craig Tyler



Digging Crystal Deep

As Los Alamos National Laboratory works to refurbish the B61 bomb—an aircraft-launched nuclear weapon it designed in the early 1960s—experimental scientists and weapons modelers are delving deep into the microstructure of TATB (triaminotrinitrobenzene), the high explosive that revolutionized the B61's safety. Unlike an earlier kind of explosive used in these weapons, TATB is extremely difficult to detonate by accident.

"You can set it on fire or slam it into a brick wall, and it won't blow up," says R&D engineer Bert Harry, who has seen conventional explosives triggered by a mere waist-height drop to the floor.

German-born Sven Vogel, a Los Alamos Neutron Science Center instrument scientist, says knowing TATB history adds meaning to his research for the B61, which is deployed in the U.S. and with North Atlantic Treaty Organization nations in Europe. In 1979, the B61 bomb switched from conventional explosives to TATB, making it the first nuclear weapon to enter the stockpile with an insensitive high explosive in the main charge. Earlier, in other bombs, some conventional high explosives had gone off haphazardly in the United States and abroad, taking lives, damaging homes, and contaminating land and water with radiation, according to declassified Department of Defense reports.

"Stories like that make clear why it is a good idea to have an insensitive high explosive," Vogel says, "and why one needs to understand how it behaves during the lifetime of a device in as much detail as possible."

TATB's discovery and rise to prominence followed three explosives accidents that killed a total of seven Los Alamos employees in the 1950s. The Laboratory pushed to create safer energetic materials, of which TATB was one, resulting in a fatality-free record since 1959. Los Alamos scientists patented the TATB manufacturing process and became the first national security lab to use an accident-resistant TATB composition in nuclear weapons.

The B61 bomb's plastic-bonded explosive, called PBX 9502, contains 95 percent TATB and was last produced commercially for the U.S. nuclear weapons stockpile in 1989. Now it's time to replenish the explosive as the U.S. Air Force and the National Nuclear

Security Administration extend the lifespan of existing B61s for another 20 years. Although the explosives won't be made at Los Alamos, the Laboratory must assess the safety, reliability, and performance of any modified weapons that enter the stockpile without nuclear testing and is responsible for the quality of updated explosives.

Producing a perfect batch of PBX 9502 could be challenging, given new production methods and new environmental regulations that dictate a different way of making the plastic binder without the harsh chemicals of the past. That's where the science comes in. "We need to characterize the existing material extremely well so we can know for certain that the replacement material is as similar as possible," says Los Alamos explosives researcher John Yeager.

When the original batches of TATB were made, not only was the science of the explosive not fully understood but weapons modelers had no way to anticipate and prepare for environmental factors, such as temperature swings or natural disasters, during a weapon's decades of service. "The codes weren't sophisticated enough to handle details at the crystal level," explains Yeager, "so certain measurements were never made."

The codes caught up in the past decade, creating a need to measure TATB's fundamental properties and to study how expected and unexpected factors could alter those properties, perhaps rendering the explosive less powerful. Such data enable new computer simulations to make detailed predictions about how the explosive will behave and when it must be replaced.

"The shape of each crystal is flat like a card," Yeager says, "so packing the crystals into a three-dimensional charge is much like trying to build a house from cards." Moreover, TATB has a rare form of crystal asymmetry. When temperatures fluctuate, the crystal structure expands unevenly, irreversibly altering the shape and size of the bulk material.

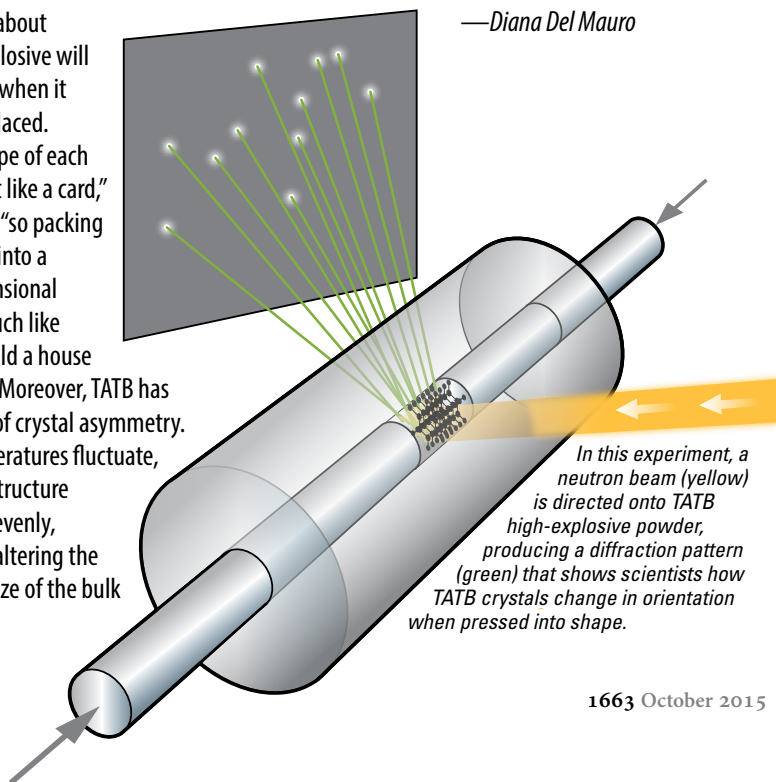
When B61 weapons modelers called on Yeager to observe and describe TATB's puzzling behavior during temperature changes, Yeager couldn't use the usual x-ray techniques, which might burn the sample when exposing crystal-level details at high resolution. With neutrons readily available at the Los Alamos Neutron Science Center, he looked to the facility's instrument scientists, including Vogel, to help him design a nondestructive approach.

Together, they collected neutron diffraction patterns from TATB powder as the explosive was subjected to cycling temperatures and compacting into charges. Their findings at the nanoscale (within the crystal) and microscale (hundreds of crystals) should clear up contradictory reports in the scientific literature and provide the "first-ever complete picture" of how the card-like crystals align during pressing, says Yeager. The data are already being fed into new computer simulations, which now account for changes in TATB properties that could occur while a weapon ages in a bunker or in off-normal scenarios, such as fire.

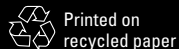
The research isn't just crucial for the B61. The latest federal guidance, according to a recent NNSA position paper, is that TATB—the only insensitive high explosive qualified for use in weapons by Department of Energy standards—should be adopted by all the nation's nuclear weapons.

A booming new era for TATB production could lie ahead.

—Diana Del Mauro



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Only moderate fire danger in the forests of Northern New Mexico? How unexpected. Most of New Mexico has been in drought since 2010, classified as severe for much of that time and accompanied by large wildfires. One year ago, less than two percent of the state was drought-free, but as of August 2015—following several months of heavy rainfall—half of New Mexico is drought-free, and less than one percent of the state remains in severe drought. Even Smokey the Bear hints at a smile of relief.

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